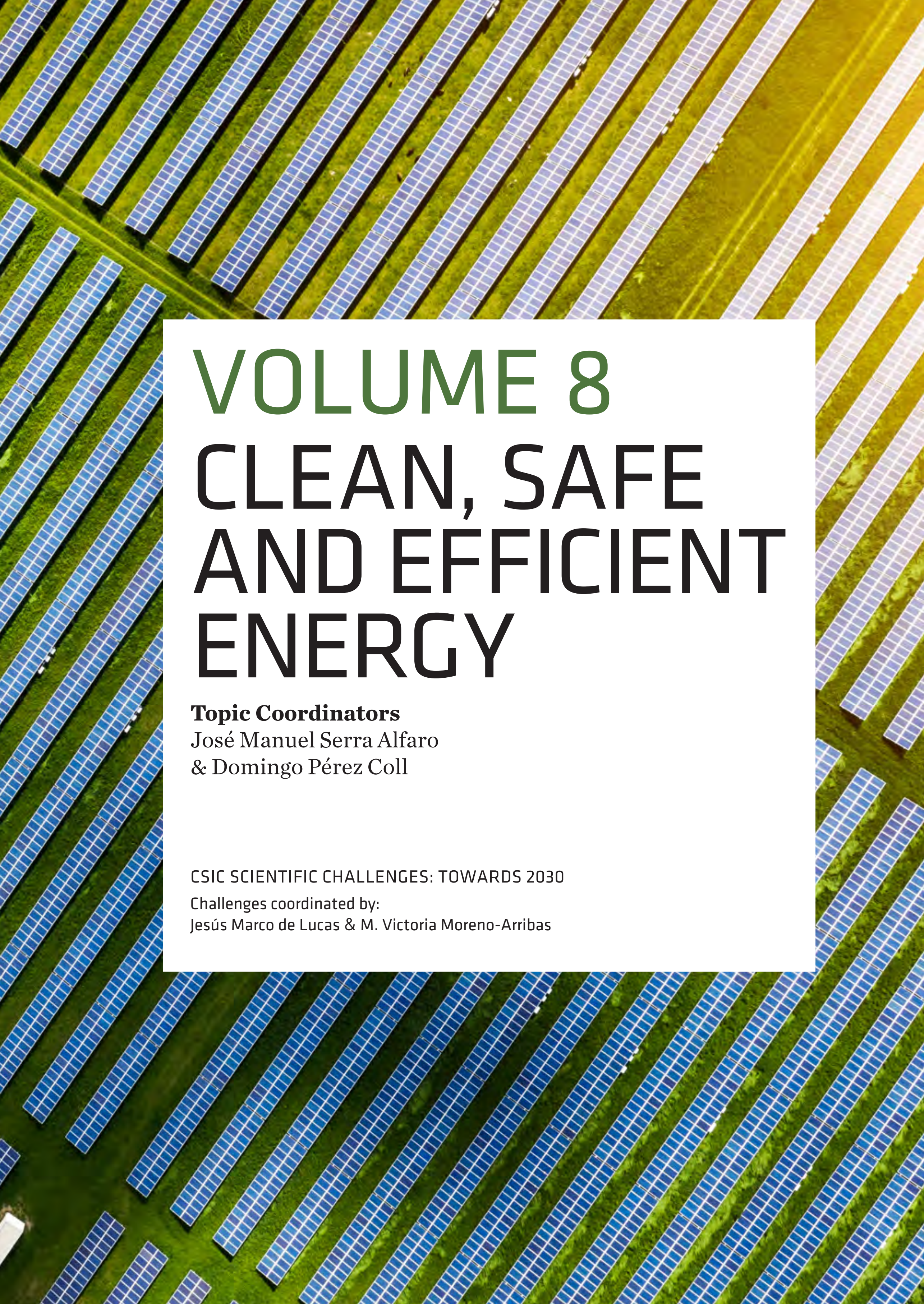

VOLUME 8
CLEAN, SAFE AND EFFICIENT ENERGY

Topic Coordinators
José Manuel Serra Alfaro
& Domingo Pérez Coll

CSIC SCIENTIFIC CHALLENGES: TOWARDS 2030

Challenges coordinated by:
Jesús Marco de Lucas & M. Victoria Moreno-Arribas

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CSIC SCIENTIFIC CHALLENGES: TOWARDS 2030

What are the major scientific challenges of the first half of the 21st century? Can we establish the priorities for the future? How should the scientific community tackle them?

This book presents the reflections of the Spanish National Research Council (CSIC) on 14 strategic themes established on the basis of their scientific impact and social importance.

Fundamental questions are addressed, including the origin of life, the exploration of the universe, artificial intelligence, the development of clean, safe and efficient energy or the understanding of brain function. The document identifies complex challenges in areas such as health and social sciences and the selected strategic themes cover both basic issues and potential applications of knowledge. Nearly 1,100 researchers from more than 100 CSIC centres and other institutions (public research organisations, universities, etc.) have participated in this analysis. All agree on the need for a multidisciplinary approach and the promotion of collaborative research to enable the implementation of ambitious projects focused on specific topics.

These 14 "White Papers", designed to serve as a frame of reference for the development of the institution's scientific strategy, will provide an insight into the research currently being accomplished at the CSIC, and at the same time, build a global vision of what will be the key scientific challenges over the next decade.

VOLUMES THAT MAKE UP THE WORK

1. *New Foundations for a Sustainable Global Society*
2. *Origins, (Co)Evolution, Diversity and Synthesis of Life*
3. *Genome & Epigenetics*
4. *Challenges in Biomedicine and Health*
5. *Brain, Mind & Behaviour*
6. *Sustainable Primary Production*
7. *Global Change Impacts*
8. *Clean, Safe and Efficient Energy*
9. *Understanding the Basic Components of the Universe, its Structure and Evolution*
10. *Digital and Complex Information*
11. *Artificial Intelligence, Robotics and Data Science*
12. *Our Future? Space, Colonization and Exploration*
13. *Ocean Science Challenges for 2030*
14. *Dynamic Earth: Probing the Past, Preparing for the Future*

CSIC scientific challenges: towards 2030
Challenges coordinated by:
Jesús Marco de Lucas & M. Victoria Moreno-Arribas

Volume 8
Clean, Safe and Efficient Energy

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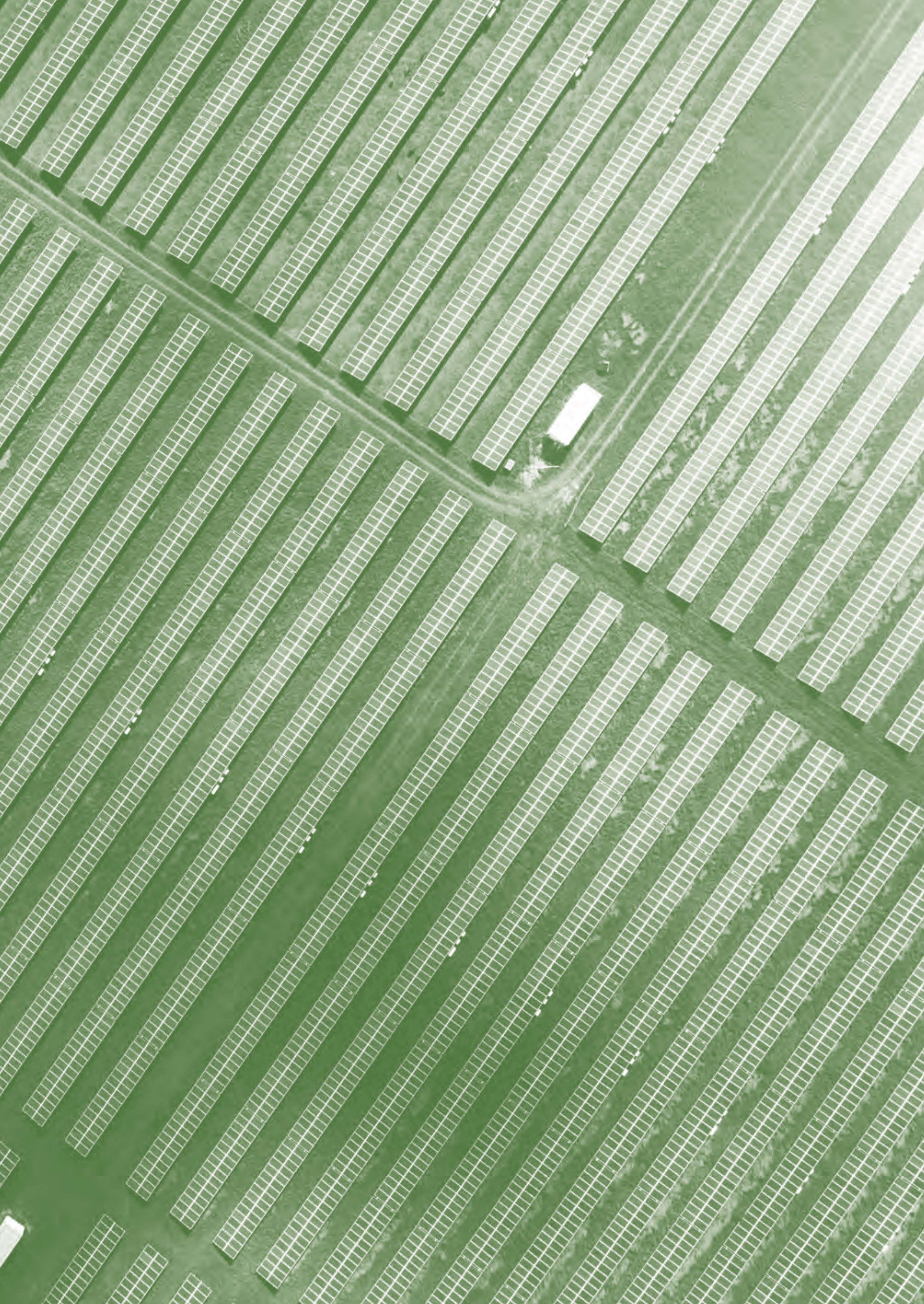

ABSTRACT

The impact of energy production by conventional technologies on the environment and human health has promoted transition policies towards a new model for the energy sector. In this context, it is essential to identify the key challenges which favour the global implementation of a clean, safe and efficient energy system, focused on the ways in which energy is produced and stored, and the management of existing resources and their emissions.

CLEAN, SAFE AND EFFICIENT ENERGY

Topic coordinators
José Manuel Serra Alfaro (ITQ, CSIC-UPV) and Domingo Pérez Coll (ICV, CSIC)

PREFACE

Contemporary society is undergoing a period of radical transformation in the way it meets growing energy demand. The gradually increasing environmental impact of conventional sources of energy production (coal, oil, gas, nuclear fission...) and its consequences on our lives is making people more aware of the need both to find alternative, clean ways to obtain power and use more efficient methods to manage existing resources and their emissions.

In this respect, public opinion around the world increasingly demands solutions to either sequestrate or stop the generation of harmful byproducts, such as the greenhouse gases causing climate change, or the toxic compounds that are increasingly affecting natural ecosystems and public health, as evidenced in the growing number of respiratory diseases in urban populations. This change of perception is reflected in the promotion of energy transition policies.

The current Strategic Theme identifies the main key challenges for the global implementation of a clean, safe and efficient energy system. Herein, we try to define the position of our institution as regards the main scientific and technical challenges that mankind will face in the coming decades in the involved fields. Our goal is three-fold. First, to identify those challenges, which will be established based on previous reports by renowned international sources and the professional experience of CSIC's experts that have contributed to the writing of this Strategic Theme. This task is prospective and, as such, implies both projection, which will be based on extrapolation of current trends, and a certain degree of educated and informed prediction. Second, to establish the current position of our institution in addressing these challenges, taking into account the work that has already been carried out and the expertise, infrastructure and human resources that are currently available. This analysis will be based on different parameters, such as scientific (research articles) and technological production (patents), as well as relevant scientific and industrial projects. Our third and ultimate goal is to make recommendations on how our institution should proceed in the future with respect to each of the identified challenges. Ideally, we will be able to devise a roadmap to consolidate or establish CSIC in a position of leadership in one or several central aspects of the Challenges. In such cases, specific measures concerning human resources, infrastructure or organizational issues will be proposed. In some other cases, our conclusion will be that the challenge should not be addressed, either because there are other actors at a national level that can tackle them more suitably, or because the effort or time required to properly position ourselves is simply too large to be realistic.

The extraordinary multidisciplinary character of the subject dealt with in this Strategic Theme required the participation of experts in very diverse fields. A full list of contributors and their affiliations can be found at the beginning of each Challenge. CSIC is expected to play an important and successful role in meeting these challenges, counting on a significant scientific network, including infrastructure and highly influential researchers in the Challenges identified in the current Strategic Theme.

The Strategic Theme is divided into nine challenges that comprise the most relevant issues ascribed to the fields of Clean, Safe and Efficient Energy. The first challenge deals with *Renewable Energy Production*, describing the key sources that provide a partial solution for the generation of clean and inexhaustible energy. Another important issue is *Efficient Energy Storage*, incorporated in the second challenge, which comprises a required group of technologies that complement the intermittency of renewable energies, enabling flexibility and distributed generation at different scales. Energy saving is a highly relevant topic as regards the preservation of natural resources, and is included in the third challenge, *Energy Efficiency and Harvesting*. Moreover, although replacing non-electrical energy, typically relying on fossil fuels, systems with electrical technologies has received much attention recently, *Industry Electrification and Grid Management*, considered in the fourth challenge, is a crucial objective for achieving full decarbonisation of industry and society. The importance of biomass as a renewable energy resource with reduced greenhouse emissions is covered in the fifth challenge, identified as *Valorization of Biomass as Energy Source*. On the other hand, the difficulty of decarbonizing several energy sectors may be palliated by the enhancement of carbon capture technologies that compensate for currently unavoidable fossil emissions, which is analysed in the sixth challenge, *Decarbonizing Energy Sectors Addicted to Carbon: CCS and CCU*. The relevance of Catalysis as a key enabling technology for many challenges in the Energy Area is analysed in the seventh challenge, *Catalysis for Industrial Production and of Energy Resources*. The last specific challenge identified in the current Strategic Theme is *Hydrogen Technologies*, and is focused on Hydrogen as an energy carrier, which represents a clean and storable solution for replacing many economic sectors based on fossil fuels. Finally, a last challenge, *Social and Environmental Aspects of the Energy Transition,* is included, which transversely relates the effect of transformation of the energy sectors considered in the other challenges on the Society and the Environment.

EXECUTIVE SUMMARY

Conventional methods of energy production are principally responsible for the generation of harmful emissions causing climate change and affecting human health. The implementation of a clean, safe and efficient energy system necessitates solutions for the way in which energy is produced and stored, and how unavoidable toxic emissions are managed. Renewable-energy production is one of the most suitable ways to produce clean and efficient energy. However, its implementation as the primary energy source requires overcoming barriers of efficiency, stability, costs and management. Not only generation of energy, but also its storage is key to introducing flexibility to the system and enabling distributed generation. Improvement in energy storage would enable generation and consumption to be disconnected, with an enormous impact on the implementation of renewable energies using the electrical grid. Portable storage technologies would also boost other electrical technologies, resulting in a drastic decrease in emission of pollutants. Energy efficiency is a further major challenge, with a direct impact on energy savings and preservation of resources. In this regard, energy harvesting presents a growing interest for technologies based on energy-autonomous electronic devices, which would enable energy to be harvested from the environment and converted to electricity. Presently, a huge amount of pollutant emissions emanates from the energy sector, complete electrification of which is complicated and directly related to the development of renewable electricity. The transport, distribution and conversion of energy in an efficient, flexible and reliable way require the development of smart power grids. Additionally, electrochemical technologies and processing of materials using electricity have an enormous potential for reducing greenhouse-gas emissions. Exploitation of biomass will provide an alternative renewable-energy source, mitigating emissions and decreasing dependency on fossil-fuel reserves. Unavoidable CO_2 emissions may be managed by carbon-capture technologies to avoid their release into the atmosphere or for use of CO_2 in different chemical processes. Technological improvements in catalysts, which play a key role in many energy-intensive industrial processes as enabling components, could decrease greenhouse emissions and toxic substances associated with energy transformation. All these mentioned challenges must be complemented with a new energy vector, hydrogen, which should be properly managed to achieve the full environmental benefits it offers. Although hydrogen may be considered as a clean and renewable fuel, its production by current technologies is highly polluting. A transformation towards its clean and renewable production will facilitate the conversion towards a hydrogen economy, in which this energy carrier could fulfil the energy requirements of all sectors of the economy. Finally, it should not be forgotten that the transition towards a clean, safe and efficient energy system and its subsequent sustainability involves a variety of social and environmental impacts which should also be the focus for research.

CHALLENGE 1

RENEWABLE ENERGY PRODUCTION

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1. INTRODUCTION AND GENERAL DESCRIPTION

The consequences of the production of energy employing conventional sources on environment and public health has encouraged the interest of the society in finding alternative methods to obtain power in a clean and efficient way. The development of renewable energy sources may be considered as one of the most suitable alternatives that can provide a solution to these problems (Directive (EU) 2018/2001). This chapter presents an analysis of the challenges and opportunities that the field of renewable energy production pose to our society. It is also about how the CSIC can contribute to tackle the former and take advantage of the latter, in order to position itself as a world leader in this field.

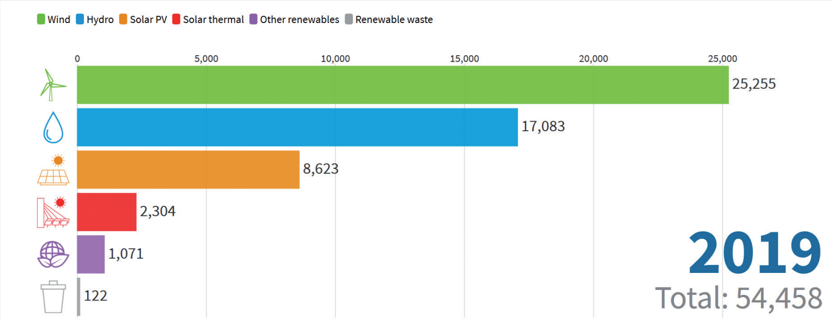
1.1. Structure of this chapter

The energy sources that will be considered under this chapter are mainly those based on the conversion of solar (section 8A.2 and 8A.3), wind (8A.4) and geothermal (8A.5) power into electricity. Other renewable sources like those taking advantage of the energy accumulated or carried by large artificial water reservoirs or rivers (hydroelectric), ocean ties or biomass are either not a subject of research within the institution, as it is the case of hydropower, or, on the contrary, the research activity carried out in our institution has been considered so significant as to devote entire chapters to them, as it is the case of biomass or hydrogen based technologies (please see Challenges 5, and 8, respectively). Also, some technologies go beyond production, as it is the case of those based on concentrated solar power, which offer the appealing possibility of storing the generated power in the form of thermal energy. These aspects will be considered in Challenge 2, focused on energy storage. In those cases in which solar energy is the primary source employed to generate some other kind of sustainable fuel, such as hydrogen, all the discussions and implications are left for the chapter specifically devoted to this fuel. Although not usually included in the list of renewable energy sources, we have included a section on nuclear fusion (section 1.6), as it is a highly promising source of clean energy. The activity in this specific field carried out in some of our laboratories is relevant enough as to deserve to be addressed specifically. The very relevant environmental and socio-economic implications of renewable energy production will be dealt with in Challenge 9. Both aspects have also political derivatives of great significance that could also be eventually addressed if this report is analyzed in an even wider framework.

1.2. Renewable Energy Sources: Current and Prospective Relevance

Approximately 15% of the total daily average consumption of energy in the world is extracted from renewable, non-polluting sources (WORLD STATISTICS). The main one of them is hydro, followed by wind, solar and the rest of renewables. In Spain, in 2019, out of the 261,020 GWh of electricity produced, 36.8% came from renewable technologies (RED ELÉCTRICA ESPAÑOLA). Spain is indeed internationally recognized as a world leader in renewable energy generation and consumption (INTERNATIONAL ENERGY AGENCY), which is the result of a robust electricity system with high shares of wind and solar PV. Unlike most other countries, in Spain, wind energy is the main source of renewable energy in terms of installed power, as shown in Figure 1, followed by hydro, and solar photovoltaics. The latter surpassed 8,000 MW of installed power capacity at the end of 2019, becoming the technology whose presence has increased the most in the complete set of electricity generation facilities, with an increase of 93,2% compared to 2018. This growing trend is shared by many other countries in the world, boosted by the need to realize a transition to a more sustainable economy.

FIGURE 1–Evolution of the renewable power installed by technologies (in MW) in the peninsular electricity system in the period 2006-2019. Source: Red Eléctrica Española.



The forecast for renewable energy technologies and markets worldwide is to be continuously reinforced. In this context, the European Union, which constitutes the political and regulatory framework that defines the directives to be followed by our country as well by all the rest of member states, is one of the most active players in the mid to long-term commitment to reach a decarbonized economy. It has established well-defined goals for 2030, such as:

1. 40 % reduction in greenhouse gas emissions compared to 1990;
2. 32 % total gross final energy consumption from renewables for the entire EU;
3. 32.5 % improvement in energy efficiency;
4. 15 % electricity interconnection between the Member States.

Out of this four goals, in two of them renewable energy plays a central role. While the third and fourth of these goals are clearly the subjects of Challenges 3 and 4, and the third one will be evidently fully included here in Challenge 1, the first one is also strongly linked to the subject of this chapter, given that a significant percentage of greenhouse gases originate in the energy system. This generic analysis reveals already the expected relevance of renewable energy production, both locally in Spain and in our nearest environment. The consecution of these goals has required from each Member State the implementation of an Integrated National Energy and Climate Plan 2021-2030, which can be consulted here in the webpage of the European Commission (European Commision).The Spanish plan is particularly ambitious and sets even higher standards than those requested by the European Commission. In fact, it aims at reaching an electricity generation based 100% on renewable energy for 2050.

1.3. Global Challenges

There are distinct generic aspects to the problem of actual implementation of renewable energy as the primary source of energy in the world. The main one is to reach the capability to *provide energy in enough quantity, on demand and at a competitive price*, just like conventional power sources currently do. The barriers towards this ultimate goal can only be overcome by improving the efficiency, stability, costs and manageability of the different clean technologies. These specific challenges have different mid and long-term implications for each one of the technologies herein considered, and will be separately addressed in each section of this Challenge.

Although all renewable energy technologies analyzed in this Challenge are, as a whole, at a very high technology readiness level, there is still a lot of room for improvement based on scientific and technical research. Further spreading of wind energy, so far the largest contributor to the electric power generation pool among all renewable power sources, requires new materials and electricity distribution networks capable of operating at extreme conditions. Photovoltaics, whose market is growing at a vertiginous pace, has still a lot of promising open routes in terms of novel materials and devices that could enormously reduce the costs of energy production and reach new niche markets such as transportation and wearable devices. Concentrated solar power offers the attractive possibility to store the energy as it is produced and, although it could also be made more efficient by improving the materials and processes involved in the cycle of energy production, its main challenge lies in the integration with other clean sources. Geothermal energy holds the enormous potential of being the only source of clean energy that is not fluctuating, but it is the less developed of them all and faces significant challenges in the efficiency of the processes required to use it, like the geographic localization of the available sources, which affects both the location of plants and distribution. All these challenges are confronted by the renewable energy community at a global scale.

On the other hand, there are other challenges that belong to the realms of sociology, politics and philosophy and that might be equally important to actually transform the world energy production into a cleaner and more sustainable one. These are, for instance: the global political response to the claim of economically emerging countries for their right to use their oil, gas and coal to fulfil their need for large amounts of energy on demand; or, the growing disbelief, many times fueled by political interests or simply based on pure ignorance, in the impartial scientific analysis and warnings of the world main threats, and, particularly affecting the subject of this chapter, in the urgency to change to a more sustainable way of generating the energy our world needs. This sort of challenges is not being addressed in this Challenge, as it will be treated separately in Challenge 9, dealing with the economic, sociological and philosophical aspects and implications of energy production and processing as a whole.

2. PHOTOVOLTAICS

2.1. Impact in basic science panorama and potential applications

The conversion of sun light into electricity through photovoltaic (PV) technology will play a major role in the energetic paradigm shift towards a decarbonized society. Indeed, recent forecasts are predicting that several tens of terawatts of PV capacity will be deployed before 2050 (Haegel, 2019). This would represent an investment of several tens of trillions of euros. A number of factors will enable the realization of this forecast, including: 1) the fact that the sun delivers on Earth hundreds of times the World's energy consumption, being PV one of the most efficient technologies to convert light into electricity; 2) the existence of an already mature technology, based on silicon, whose cost is reducing very rapidly; and 3) the springing of myriad emerging PV families that are meant to enhance the performance of the existing technologies or broaden the PV deployability.

Current research trends are ultimately related to the sun being a source of abundant but dilute energy compared to chemical energy stored in fossil fuels. As a consequence, vast areas need to be covered with PV panels in order to harvest enough energy to match present and future demands. This already implies the use of abundant and non-toxic raw materials with as low as possible embodied energy. For the conventional technologies, this means that reducing embodied energy and/or increasing efficiency are very attractive development avenues. In the case of the emerging technologies, they would find a market beyond niche applications if they exhibit a significantly enhanced efficiency, or, alternatively if they can complement or extend the range of applicability of silicon.

Currently, most PV is deployed as solar farms. In the midterm, PV will be both centralized in more efficient farms and distributed throughout constructed land. They are expected to power portable devices, to be part of urban furniture, or to be integrated in buildings (BIPV), awnings, roads, vehicles, clothes, bags... This vision will become true as more versatile technologies reach the market. Traits of some future PV technologies include low cost, short energy payback times, semitransparency, flexibility, color tuning, camouflage appearance, lightweight, or hardness. In the long run, sustainability will increasingly become the dominant factor for the development or choice of PV technology.

Consolidated Technologies

There are a number of photovoltaic technologies whose development started in the 1970s and that are currently commercially available. These include PV based on crystalline silicon heterostructures (luminous to electric power conversion efficiency: 26.7%), single-junction GaAs (29.1%), CIGS (23.4%), CdTe (22.1%) and stabilized amorphous Si:H (14.0%), with the number between brackets being the corresponding certified lab-scale record power conversion efficiencies [source: NREL chart, accessed on the 10th of March 2020], see Figure 2. Crystalline silicon (c-Si) is an indirect bandgap semiconductor, which results in a weak absorption that has to be compensated by very thick active layers. This motivated the search for alternative direct semiconductors that could be designed as thin films, and thus technologies based on CIGS, CdTe and Si:H were born. These technologies require less semiconducting material and lower processing temperatures, which leads to lower energy payback times compared to crystalline silicon. However, CIGS and CdTe are based on materials that are toxic and/or scarce. The most efficient single junction solar cells made to date is based on GaAs (generally speaking, III-V semiconductors), which is also the base for multi-junction solar cells that have reached efficiencies above 47% under concentration. As the cost is significantly higher than that of silicon, GaAs based PV has so far found mainly niche applications.

Despite the variety of technologies, crystalline silicon dominates the current PV market. The competitive advantages, given by a large production volume and decades of technological refinement, place silicon PV in a position that leaves little room for competitors attempting to offer lower prices. Silicon wafer cost currently represents 8.6% of utility system costs and an even smaller fraction of the levelized cost of energy. While the current efficiency record for silicon solar cells is 26.7 %, state of the art commercial silicon modules have efficiencies just above 20%. Silicon modules can also be made bifacial with a negligible increase in fabrication cost but with an energy production up to 30% higher by harvesting the backside light reflected from the ground.

Emerging photovoltaic technologies

Given the current cost and performance of crystalline silicon, do we need other technologies? Despite the very impressive cost reduction and further efficiency optimization, crystalline silicon has a number of fundamental limitations that restricts its potential uses. First, the non-optimum electronic bandgap of Si appreciably limits its maximum efficiency unless tandem structures are designed. The efficiency is also severely affected by temperature, or by light impinging at non-normal incident angles. On the other hand, so far Si PV can only be made semitransparent by leaving gaps between cells (or drilling holes through it), and color can be tuned by using filters, both of which have strongly detrimental effects on the resulting efficiency. Moreover, silicon is heavy and brittle, which prevent its use where flexibility, lightweight or mechanically robust materials/structures are needed. Finally, the high temperatures needed to produce crystalline Si result in an unavoidably large embodied energy. So a number of technologies are being developed trying to tackle (some of) these issues.

Inorganic cells that build on the knowledge from CIGS use abundant and low toxicity materials, such as Cu_2ZnSnS_4(Se), and currently reach efficiencies up to 12.6%. Quantum dot based cells are often processed from solution at low/moderate temperatures, which is an attractive trait. While the latter has led to lab scale cells exciding 16.5% power conversion efficiencies, the attempts to remove the undesirable lead have thus far resulted in much poorer performance. Technologies based on organic materials, also known as excitonic photovoltaics, include a plethora or subclasses, such as dye sensitized solar cells, evaporated small molecule, and solution processed binary/ternary bulk heterojunction photovoltaics. The latter has experienced a recent boom with the continuous synthesis of novel compounds that have taken their efficiency up to 17.4% (uncertified over 18%), while using non-toxic materials. Interestingly, organic photovoltaics promise very short energy payback times as well as the possibility to tune color, transparency and flexibility. They suffer, however, of poor stability thus far, and present an efficiency that should also be improved further. More recently, hybrid organic/inorganic lead halide perovskites have attracted a well-deserved attention as their performance has gone from less than 10% to the current 25.2% in less than ten years, which is an impressive value for a solution processed technology. Efforts in this case are placed on the replacement of Pb, improving stability and hybridizing with c-Si cells in multi-junction devices. Finally, other technologies are also appearing, such as solution processed all-oxide cells, which promise enhanced intrinsic stability and compatibility between different layers of the cell stack. Moreover, some oxides are ferroelectric, which could theoretically be through the so called bulk photovoltaic effect (<8% efficiency so far).

2.2. Key challenging points

The European Commission, after consultation with many stakeholders, established a SET Plan for the development of photovoltaics (SET, 2016). The SET Plan established a series of ambitious goals for the PV technology in terms of efficiency, cost, sustainability and integration.

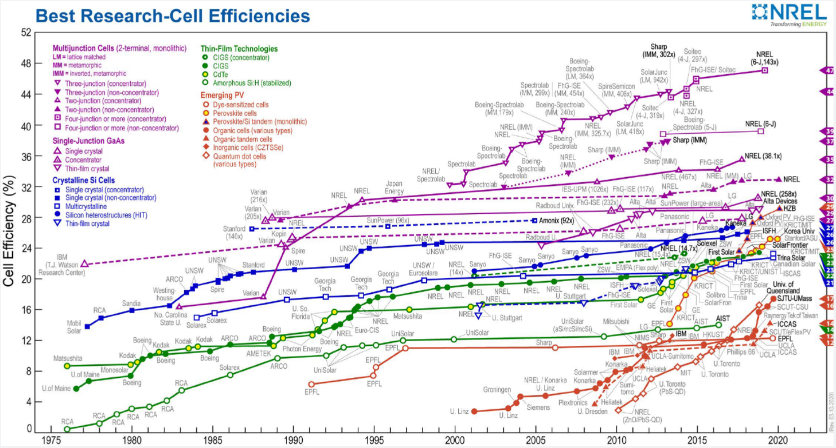
Efficiency

The goal of the SET Plan is to increase in 35% the PV module efficiency by 2030 compared to the values in 2015. This target is set for both commercial technologies (c-Si, CIGS, CdTe) and new concepts. The capacity of a PV installation is the product of many factors (cell efficiency, inverter efficiency, tracking, optical efficiency). The trends towards higher efficiency in each one of these factors reinforce the others in a synergistic nonlinear positive feedback loop. The nominal standard efficiency of modules in utility-scale new installations is increasing by 0.6% per year on average. At the current rate we will reach the practical limits of single junction photovoltaic technology within a decade, noting that 80% of the U.S. utility-scale systems installed in 2016 already used tracking. A similar trend towards higher inverter efficiencies has also been reported.

The only proven method to significantly increase the c-Si efficiency beyond the limits of conventional technology is the use of multi-junction devices. Making a realistic estimate including temperature and spectral variability effects, it has been shown that the energy production of a silicon solar cell can be increased by 23% by stacking on top of silicon a semitransparent solar cell with an absorption threshold (band gap) of 1.69 eV [Ripalda, 2018]. Strong efforts are placed on the fabrication of tandem cells hybridizing silicon and halide perovskites as well as quantum dot technologies.

Perhaps motivated by the current climate emergency, by scientific policies attracting researchers to the field and/or by the market pressure resulting from

FIGURE 2—NREL research cell efficiency chart for different technologies, accessed on the 10th of March 2020.



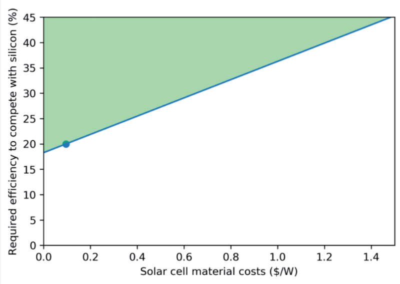
the advent of hybrid perovskites, most technologies have experienced a significant increase in certified efficiency values over the past five years. This is true for both conventional and emerging technologies, the only exceptions being amorphous silicon and dye sensitized solar cells (DSSC).

In the short term, demand for emerging PV technologies can be expected if these can exceed the efficiency of silicon single junctions or provide alternative benefits (see below). It is worth noting that the cell efficiency of multi-cation hybrid perovskite has rocketed up to values above 25% in one decade, a value that is already higher than those for multicrystalline and thin-film crystal silicon cells. Strong efficiency improvements at cell level have also been witnessed by both quantum dot cells and organic photovoltaics, currently exhibiting around 17%.

Cost

The SET Plan aims at reducing “turn-key system costs by at least 50% by 2030 compared to 2015 with the introduction of novel, potentially very-high-efficiency PV technologies manufactured at large scale”. The current cost structure for a large scale PV system is 0.10 $/W for silicon wafers, 0.25 $/W for other components and costs in PV modules, 0.21 $/W for support structures and trackers, 0.06 $/W for power electronics (inverters), 0.04 $/W for land

FIGURE 3—The green shaded area represents the parameter space of PV technologies competitive with silicon in terms of dollars of capital investment per peak watt of capacity. The blue dot is the current status of commercial silicon PV technology.



acquisition, and 0.45 $/W for balance of system costs (taxes, profit, margin, minor expenses) (Fu, 2017). Thus the cost of PV generated electricity is now mostly determined by costs other than that of the device itself. In this context, increasing the energy efficiency not only results in a higher return on investment, but also lessens the environmental impact of PV installations. The second consequence of such cost structure is illustrated in Figure 3, where the green area is the parameter space of PV technologies competitive with silicon in terms of dollars of capital investment per peak watt of capacity. Clearly, emerging technologies should combine sufficient efficiency with the use of abundant materials deposited through processing schemes exhibiting low thermal and vacuum budgets in order to become competitive technologies. While many of these factors have been proven for some of the emerging technologies at cell level (e.g. hybrid perovskites and organics), upscaling is still work in progress.

3. CONCENTRATED SOLAR POWER (CSP)

3.1. Impact in basic science panorama and potential applications

A concentrated solar power (CSP) plant generates electrical energy with a thermal power block that uses the heat produced by concentrating the sun irradiation by means of mirrors or heliostats. Three main designs are commercially used: (i) parabolic trough power plant, (ii) power tower systems and (iii) linear Fresnel technology. Currently, the installed capacity worldwide is around 5.5 GW (Concentrating Solar Power Projects, 2019) [Source: National Renewable energy laboratory (NREL), "Concentrating Solar Power Projects," 2019.], whilst the roadmap proposed by the International Renewable Energy Agency (Remap Case 2050) estimates an ambitious total installed capacity of 633 GW by 2050 (Solarpace, 2020) [Source: Global Energy Transformation - A roadmap to 2050. IRENA, 2018]. Thus, a huge deployment of CSP technology is expected. Spain is leader in concentrated solar energy production with 50 operating plants with 2.3 GW cumulative capacity (Solarpace, 2020). Most of them (45) are parabolic trough, while three are power tower systems and two have linear Fresnel technology. Moreover, the first commercial power tower plants in the world were constructed in Sanlúcar la Mayor (Sevilla), PS10 in 2007 and PS20 in 2009, with 11 y 20 MW, respectively. Places such as the US, Southern Europe, the Gulf region, Chile and South Africa have a great potential for concentrating solar power (Lilliestam, 2018). According to the international energy agency a total of 40 projects are to be commissioned over the next five years (IEA, 2020). Most projects, 21, will be towers, followed by 15 parabolic troughs and 4 linear Fresnel technology. Moreover, projects will grow, typically greater than 100 MW to benefit from economy of scale.

A concentrated solar power plant consists of the basic following elements: (i) solar field, (ii) receiver, and (iii) thermal power block. The total efficiency of the plant is the product of the efficiencies of the different elements. Thus, it is determined by the optical, receiver, and power block efficiencies. Moreover, these efficiencies depend on concentration ratio and receiver temperature (Cahen, 2017). Therefore, increasing the plant efficiency implies increasing the concentration ratio and/or temperature. Nevertheless, it should be also considered that technologies for increasing efficiency might lead to an increase in construction costs that should be taken into consideration. CSP electricity price is currently higher than that obtained from PV, but CSP has the possibility of incorporating a thermal energy storage unit to produce electricity even without solar irradiation (dispatchable renewable energy technology). Thermal energy can be stored as sensible, latent, or thermochemical heat. Storage of heat is nowadays cheaper than storage of electricity. Moreover, new solutions are expected that couple CSP thermal cycle to other applications such as water desalination systems.

In recent years, the high cost pressure and industry development produced significant cost decrease and learning rates increasing 20%. Such trend is expected to continue in the near future (Lilliestam, 2017). Significant efforts have been done to reduce the electricity cost of CSP with the goal of being competitive with conventionally generated electricity without subsidies. The EC H2020 program has recognized the importance of research focused on this cost reduction. Thus, in the Work Program it is specifically stated that it is needed to "improve the competitiveness of the CSP technology, by demonstrating cost reductions and increased performance and reliability of CSP plants, therefore strengthening the European industrial sector and improving the prospects for CSP deployment in Europe". There are 26 active H2020 projects within CSP topic. The same objective is shared by the SunShot program from the Department of Energy of the USA government. Within the targets of such program is the aim of reducing the cost of electricity by an additional 50%, to 5¢ per kilowatt hour for dispatchable CSP, between 2020 and 2030. Based on these further cost reduction in CSP, for countries with high solar irradiation such as Spain, a high development of complementary photovoltaic and CSP plants is expected, as they are economically more interesting than the integration of electricity storage or fossil back-up systems (Pitz-Paal, 2017).

3.2. Key challenging points

The European Solar Thermal Electricity Association set a strategic research agenda 2020-2025 for the development of the CSP energy (ESTELA, 2012, 2016). In this agenda detailed research topics and related targets for this industry are presented for the next future. Three main objectives have been proposed which serve to identify the main global challenges that the technology poses:

Challenge 1: Increase efficiency and reduce generation, operation and maintenance costs. In order to reach this goal, the development of novel materials that could outperform currently employed ones has been identified as one of the key achievements that will lead to a more efficient CSP technology. More specifically: new advanced mirrors, with improved reflectivity and durability (antisoiling coatings); new receivers, made of selective coatings with better optical properties and new engineered materials capable of standing higher temperatures; new heat transfer fluids, based on low melting temperature mixtures or pressurized gases, as well as absorber tubes that can stand higher pressures and direct the steam generation. Other challenges to improve the technology belong to the realm of engineering, such as new conversion cycles and systems, which require advanced power cycles and thermal storage system integration schemes or advanced hybridization schemes with other renewable energy sources. It is also relevant to improve control, prediction and operation tools.

Challenge 2: Improve dispatchability, which implies hybridization and integration systems, and in particular integration with large steam plants, with gas turbine and combined cycle plants, or with biomass or PV plants. Also, it involves hybridization, for the direct systems, using the same molten salt mixture as high temperature fluid and heat storage medium. This objective also covers advances in storage, which is one of the most attractive features of this technology, a concept that will be further detailed in Challenge 8B.

Challenge 3: Improve Environmental Profile. It is worth describing some of the solutions that are currently being explored and might indicate the path to go for the next decade. One of the most actives and promising fields of research affecting CSP technology is that of outstanding solar-thermal absorbers. Sophisticated solutions such as three-dimensional structured graphene metamaterial (SGM) have been recently proposed (Lin, 2020). Moreover, significant efforts are being done in raising the temperature of the process to increase efficiency. In commercial CSP plants, the state of the art is the use of molten nitrates with maximum working temperatures limited to about 565 ºC, as both heat transfer fluid and heat storage material. The thermal decomposition of nitrate salts can result in changes in their composition or potential risks of NOx emissions. So, there is also active research to propose new fluids for higher temperatures. In this field new proposals are expected by using more complex mixtures with larger operational ranges of temperatures and improved thermal properties such as higher thermal conductivity. Moreover, new corrosion studies are required as experimental conditions of use are quite harsh. Proposals of new materials or coatings will be also needed.

4. WIND ENERGY

Energy harvesting from wind is one of the most extended and implemented renewable energy sources. Accordingly, it is expected to be the largest contributor to the energy target planned in the SET-plan. In Europe, wind generation power achieved 169 GW at the beginning of 2018, almost 16 GW being offshore and 153 GW onshore. By 2020, it is expected to achieve 210 GW, supplying 14% of the global demand. By 2030, it expected to grow up to 350 GW from which 70 GW would be offshore, thus achieving up to 30% of the power demand (SET, 2018). Remarkably, in Spain, during 2019, out of the 36.8% penetration of the renewals achieved in the pool of energy of the electrical system, 20.6% corresponds to wind (REESA, 2020).

The high expectations for the implementation of wind energy as a reliable and cost competitive energy resource integrated in the grid has led to the opening of an attractive market and, simultaneously, has set significant and numerous challenges. This interest was based on the advantages of the wind technology in terms of reliability, long and efficient life, low investment and maintenance costs, and low environmental impact. In turn, the intrinsic irregularity of energy generation based on wind, requires the development of specific strategies and technologies to adapt the electrical grid.

4.1. Impact in basic science panorama and potential applications

Inland

The evolution of wind generators in the last decades, specially for inland installations, has been based on the power production of each unit. In the last generation, a typical power of 2-3 MW per unit has been achieved, being the power limited by the impact of the large size of the blades of the turbine blades and the inconstant blowing regime of the wind, as well as by the requirement of an optimization of the LCOE (Levelized Cost Of Energy) concerning maintenance and investment costs. The production of wind generators attends industrial criteria to minimize costs of civil works, transport and installation. From the point of view of the selection of the site, additional requirements are: an adequate averaged wind speed and the proximity of electrical connections to grid with enough capacity to drain the power generated. The so-called wind farm includes all the items required for the connection to the grid, and this pattern is reproduced by all manufacturers and investors. There are more than 100 manufacturers worldwide that warrant a competitive market. Most of them operate and manufacture in Europe: Siemens-Gamesa, Vestas, General Electric, Enercon, Nordex, Goldwind, Suzlon, etc. Each one accumulates more than 10.000 operating generators, the first of this list surpassing already 50.000 units.

Although the market has a high level of competence, and the technologies do not differ in a high degree, there is room for innovation and development to diminish the maintenance costs, increase the operating time and life time, diminish their carbon footprint, and avoid the extensive use of the so called strategic raw materials. All this research and innovation is required if we want wind energy to be a major player within the future energy systems.

Off-shore

Major advantages of wind power generation by off-shore farms are the available room for large turbine blades and the constant blowing rate of the wind.

These advantages have pushed the manufacturers and investors to consider building wind generators of higher power, but pose several challenges associated to the structure of the wind generator, which must be adapted to strong winds, the extreme conditions of the wet and salty environment, the low temperatures, and the few days that the generator can be accessed for maintenance and building up. The development of 10 MW wind turbines is now achievable.

An additional shortcoming concerns the link of the remote placement of the wind energy collectors in off-shore plants with the land grids. This requires the development of specific sea networks able to concentrate the energy in farm nodes that, acting as energy islands, enable energy transport to other nodes and lines in the land. New power electronics developments, functionalities based on the unique properties of high temperature superconducting (HTS) materials and the development of procedures for an effective environmental protection and anti-icing functions, are new strategies to be deployed to cope with the requirements of a safe and efficient off-shore operation. New devices based on the unique performances of the superconducting materials, such as fault current limiters, simplified electric generators able to work at low rotational speed in direct connection to the turbine or robust systems for energy storage to prevent short time failures, and cables with ultra-low impedance are presently being tested. HTS materials are now produced in 100's of kilometres per year, being the cost one of the most relevant challenges for the application.

4.2. Key challenging points

Despite the apparent maturity of wind generators, the two essential elements, generator and grid integration, are in continuous development. In what follows, we identify a series of technical challenges affecting the performance of the generator and other parts of the windmill, as well as others aspects specifically related to grid interconnection, although this matter will also be dealt with in Chapter 8D, focused on electrification strategies.

From the research point of view, the field requires efforts to develop materials with specific electrical and magnetic properties in order to lightening the mill structures and enabling the construction of larger and more efficient generators. It also demands the development of new devices to improve the grid resilience. In addition, the development of materials to ensure continuous operation in extreme conditions during long time and efficient forecasting models for optimization of resources and minimizing environmental impact should be promoted following the trends developed by the European Green

Deal. Key points regarding these issues encompass the following aspects: i) regarding the generator, simplification, reliability, improve efficiency, decrease inertia, reduce maintenance cost and expand the time between maintenance actions; ii) concerning the turbine, decrease corrosion and improve anti-icing or de-icing functions in extreme conditions, that call for the development of improved materials and functional coatings; and iii) regarding grid integration, improvement of wind forecasting and energy storage and management procedures, in order to apply reliable predictive models.

Although incremental improvement in these aspects is expected by the application of current technologies, breakthroughs are still expected through the incorporation of radically new technologies based on HTS materials. This will be the case for the design of novel current limiters, transformers, and hybrid energy storage systems as SMES to enhance power and safety of the grid and to protect the generator against electrical events. For this, it is mandatory to reduce the HTS materials cost and increase their production capacity and strong efforts are being devoted to prepare HTS tapes with a low cost/performance ratio (Puig, 2020). Other issues, where the incorporation of HTS solutions can be an option with respect to standard alternatives based on permanent magnets, concern the system design and aim at diminishingthe weight of the generator and its kinetic moment, at increasing the power density and to apply the concept of "direct drive" or medium speed to avoid or diminish the complexity of the gear box. HTS also allows facing the impact of the critical raw materials required by the permanent magnet alternatives. All these call for an improvement in HTS manufacturing procedures and costs, magnetic field behaviour of the critical current, homogeneity of the wires, quench resilience and in mechanical properties, topics that are matter of research challenges nowadays.

In wind farms located off-shore and in other placements with aggressive environmental conditions, emerging problems deal with the effect of salty water, the usually stronger wind and the low, very frequently minus zero, temperatures that lead to increasingly higher maintenance costs. Formation of ice aggregates on the blades and other components may be a critical problem in cold climates (Golovin, 2013). The foreseen progression in the installation of wind facilities in locations where corrosion is very severe makes the finding of protection solutions and in-place analytical monitoring techniques critical to reduce the environmental impact (Kirchgeorg, 2018). Innovative surface engineering solutions, in-situ and automatic monitoring and alarm systems will be some of the future developments that will be implemented to reduce aging of the facilities and derived environmental deleterious effects.

5. GEOTHERMAL ENERGY

Geothermal energy utilizes the heat from the Earth interior to produce electricity and/or deliver heating and cooling. The highest heat gradients are found around tectonic plate boundaries and in active volcanic areas. A remarkable characteristic of this renewable energy is its capacity to provide a constant output of energy if required. Thus, geothermal energy can cover the base of smart thermal and electricity grids. However, only a small portion of the geothermal potential is currently being exploited, leaving a huge potential for further deployment ahead (Bertani, 2016). Geothermal energy can be classified into power generation and/or direct use of heat. Power requires of high enough temperature to boil a fluid to move turbines. Once the fluid condensates, its heat can still be used, maximizing efficiency. Heat can also be used in a cascade way, using it in various applications that require a progressively lower temperature, to enhance efficiency (Shortall, 2019).

5.1. Impact in basic science panorama and potential applications

The global installed capacity of geothermal power plants is 11 GWe, 3 GWe of which are installed in Europe in 127 geothermal power plants (Uihlein, 2018) (Dumas, 2018). Geothermal energy represented the 6.8 % of the energy supplied by renewables in 2017 (IEA, 2018). 93 % of the installed capacity worldwide is concentrated in ten countries: United States, the Philippines, Indonesia, Turkey, Mexico, New Zealand, Italy, Iceland, Kenya and Japan. Currently, Spain does not produce electricity from geothermal energy. The generalization of the use of geothermal energy for heating and cooling purposes can significantly contribute to reach carbon neutrality (HEAT ROADMAP EUROPE, 2019). If the geothermal power development targets of all countries are met, the installed capacity would reach 32 GWe in 2030 (Matek, 2016). Furthermore, it is estimated to scale up by one order of magnitude by 2050 provided that research and development comes up with innovative solutions for reducing the current pre-development costs and high risks (Limberger, 2018) (De Simone, 2017).

5.2. Key challenging points

To generalize the use of low-enthalpy geothermal systems to climatize buildings. Representing half of the total energy demand, building climatization through heating and cooling requires to undergone a profound transformation to decarbonize the sector and achieve near Zero-Energy Buildings (nZEB). Geothermal energy is a ubiquitous renewable source and, as such, it can be used anywhere in the planet for heating and cooling purposes through Ground Source Heat Pumps (GSHP) and Underground Thermal Energy Storage (UTES).

To lower the temperature required for generating electricity from medium-enthalpy geothermal systems. Such achievement would imply generating electricity at shallower depths, facilitating operations because permeability of geological media usually decreases with depth. Furthermore, it will enable the combination of geologic carbon storage with geothermal energy production.

To attain enhancing permeability in tight rock for high- and very high-enthalpy geothermal systems. Deep geothermal systems rarely present enough permeability to be operated without having to stimulate the wells. Effective stimulation techniques with a low induced seismicity risk should be developed to permit enhancing reservoir permeability without inducing large earthquakes. Improving zonal isolation is key to stimulate individual fractures in a controlled way, rather than stimulating the whole open well simultaneously. Combination of hydro-fracturing and hydro-shearing should permit creating a reservoir permeable enough to circulate fluids between the doublet of wells without imposing an excessive pressure gradient.

To mitigate corrosion and scaling issues caused by the high reactivity of chemical species in high temperature environments. Geochemical modelling can assist the operators of geothermal plants to set the optimum operating conditions in order to minimize corrosion problems and clogging due to scaling. Such issues imply elevated maintenance costs and replacing equipment, like pumps. Methodologies to reduce these problems as well as potential ways of utilizing precipitated minerals will be necessary as geothermal energy scales up.

To forecast induced seismicity in order to minimize the risk of inducing perceivable and damaging earthquakes as a result of geothermal energy production. Forecasting injection-induced seismicity is a big challenge that will require of ground-breaking solutions. Current protocols have proven unsuccessful and thus, a new paradigm is required.

6. FUSION: AN ALTERNATIVE CLEAN ENERGY SOURCE

Fusion energy has been, since many years, a promise of unlimited, safe and carbon-free electricity energy source. Fusion is a source of heat-related generation route, which could become a base load of electricity source or even an energy source for renewable fuels (Hydrogen for instance). The most suitable nuclear reaction for fusion reactors is D + T = He + n + 17.6 MeV, where D is deuterium and T tritium. Since the concentration of deuterium in the oceans is rather high and tritium can be generated through the nuclear reaction of neutrons with Li, there exists enough fuel to generate the energy required for mankind for millions of years. This reaction, however, requires a temperature (T) in the range of 100 millions degrees and to achieve a plasma density (n) high enough to overcome the Coulomb repulsion during a long enough time.

6.1. Impact in basic science panorama and potential applications

Historically, the progress towards the fusion goal made a quantum leap with the design of tokamaks as magnetic confinement systems for plasma. Initiated in the Kurchatov Institute in Moscow in the late 60's, since then several tokamak models have been built and plasma properties for fusion were tested all around the world. All this R&D led to the largest international scientific installation ever organized (35 countries, a cost of at least 10 bn€ in 30 years of life), the International Thermonuclear Experimental Reactor (ITER). ITER is nowadays under construction in Cadarache (France), ignition should start in 2023 and its design is based on the best materials available in the early 2000s. ITER is an experimental reactor, still not intended to generate usable energy. Electricity is instead scheduled to be generated in the next prototypes, the so-called DEMO reactors, being at present in the initial stage of design in several continents (Europe, Japan, China, …) and which should incorporate novel materials and technologies. Overall, these "classical" fusion technologies based on low temperature superconductor (LTS) materials are expected to generate clean energy beyond mid-21st century.

A game changer appeared just after ITER was designed in 1986: high temperature superconductors (HTS) and the development of high magnetic field conductors based on $REBa_2Cu_3O_7$ coated conductors (REBCO CCs, where RE stands for Rare Earth or Y), which allowed the development of ARC (Affordable, Robust, Compact) tokamak reactors (Sorbom, 2015). HTS magnets are expected to generate magnetic fields of 12 T at the center of plasma, compared to the 5 T of ITER, which has a huge effect on the energy gain that can be achieved with a fusion reactor, which is proportional to ~ B^3 while the power density is ~B^4. As a consequence, ARC compact reactors (~500 MW) have a core radius of 1.5 m instead of 6.2 m of ITER and the overall plasma volume is 10 times smaller (Whyte, 2016).

A key issue of ARC reactors, besides the smaller size and the lower cost, is the long term life expectance. While in ITER replacing any material in the core becomes a tantalizing technological problem involving very complex robotics, ARC reactors are much more compact and demountable, thus making accessible the inner vacuum vessel for any replacement. This novel design has an enormous impact in the long term requirements on materials and engineering devices of the fusion reactors, particularly it reduces the concerns on irradiation effects by enabling spare replacements.

ARC fusion reactors are, therefore, a very recent breakthrough requiring still intensive R&D of materials and plasma physics, but they have the potential to bring fusion energy to reality much sooner and much cheaper. First estimates and technological development plans of the novel spin-off companies (for instance, Commonwealth Fusion System in US and Tokamak Energy in UK) is that 2030 is a reasonable horizon to have net fusion energy generation. Fusion energy appears again, therefore, as a unique opportunity to become a clean energy source in a reasonable time scale.

6.2. Key challenging points

There are many scientific and technical challenges associated to the compact fusion reactors, many of them related to the relevance of neutron (14.1 MeV) irradiation effects on the vessel, magnets and other advanced materials around the core of the reactor. But even if these issues are significant, the most relevant challenge is to further improve the performance of REBCO CCs and the corresponding magnets.

The requirements related to CCs are multiple because tokamak reactors are composed of different magnets working under different physics conditions. Some of them are:

- Achieving high critical current densities under these extreme conditions; this is a very challenging objective which is even stronger when we consider that low cost manufacturing techniques are needed to obtain competitive km-long conductors.

- Achieving a high figure of merit cost/performance (€/kA m, i.e. cost of 1 m of CC having 1 kA of critical current), needed to advance in low cost chemical methodologies, such as Chemical Solution Deposition (CSD), and high throughput production (fast growth techniques) of REBCO CCs (Obradors, 2014).
- Development of efficient stabilization architectures against quenching, since lifetime of magnets depend critically on the fast propagation of quench.

In conclusion, among the demands of R&D related to compact ARC fusion reactors we should consider many issues related to the plasma handling and materials working under extreme conditions, but the technological development of HTS materials and magnets stands as the most relevant challenge.

7. CONCLUSION

From all the facts and figures presented in this chapter, it can be stated that our country is called to play a key role in the future development and commercialization of renewable energy. We have natural resources, a high level of technological advancement already achieved and the international recognition of our position in this field at all levels. There is, therefore, a clear opportunity to overcome the endemic and historical dependence of our economy on highly fluctuating activities such as tourism and construction and try to establish ourselves as world leader in a technological field. Coordinated efforts devoted to renewable energy by all potentially contributing national actors should be highly encouraged. In this context, CSIC have all the potential to become a central piece in this picture if proper planning and allocation of resources are in place.

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Section 6. Fusion: an Alternative Clean Energy Source

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TABLE 1—List of challenges to be addressed for the Challenge 1

	SHORT TERM (< 5 YEARS)	MID TERM (5-10 YEARS)	LONG TERM (> 10 YEARS)
PHOTOVOLTAICS	• Create a CSIC PV technology platform as a vehicle to communicate and find synergies between PV technologies. Position CSIC as expert on PV related topics at national/ international levels. • CSIC to consolidate links with the most relevant energy institutes working on PV • Proof of concept hybrid photovoltaic technologies based on two PV technologies. • IP protection and dissemination of novel device concepts, materials and processing protocols. • Determination of main factors limiting device stability in the different technologies. • Demonstration of emerging solar cell technologies with high efficiency and durability for small scale applications (e.g. powering IoT) • Rise public awareness of the energy problem.	• CSIC to gain critical mass on priority PV topics. Possible creation of a CSIC Institute of Energy Research to unify efforts in a multidisciplinary approach to the energy challenge. Coordination of a European Energy Flagship (international leadership). Cooperation to reduce non-PV related cost of the systems. • High efficiency solar cell technologies with no scarce or toxic elements. • Demonstrated long term stability for selected PV technologies. IP protection on encapsulation strategies. • Demonstration of ultrahigh PV efficiency >50%. • Proof of concept hybrid PV/ non-PV technologies. • Achievement of high TRL for novel concepts that facilitates a wide deployment of building integrated photovoltaics. • CSIC/Industry co-development of upscaling and manufacturing process for selected PV technologies.	• CSIC to exploit the generated intellectual property on PV. • Demonstration of solar cell technologies with energy return on investment greater than 50 for unrivaled energy generation sustainability. • Achieving high TRLs for hybrid concepts with very high efficiencies. • Availability of a large palette of efficient and durable solar cell technologies to enable nationwide deployment at all levels (solar farms, buildings, public infrastructure, designs, textiles, advertisement infrastructure, portable devices, vehicles, etc.). Wrapping cities on PV.

	SHORT TERM (< 5 YEARS)	MID TERM (5-10 YEARS)	LONG TERM (> 10 YEARS)
CONCENTRATED SOLAR POWER	• Development of new high temperature range (low melting point and high stability temperature) fluids • Development of nanofluids with improved thermal properties (heat capacity or heat conductivity	• Developments in Latent and sensible heat storage systems (achievement of higher TRL) • Development of new receiver materials and coatings with high absorptivity and high thermal stability • Studies in Materials compatibility with new thermofluids • Advanced solar mirrors • Integration with high temperature power cycles • Global CSP systems cost reduction (LCOE 5-7 c€/kWh)	• Integration of CSP with other technologies (such as water desalination) • Achievement of high TRL of new thermochemical storage systems • Hybrid systems integration (such as CSP/PV)
WIND ENERGY	• Improve passive and active de-icing systems and their integration in blades and other components • Development of new low-weight structural materials for the building of lighter structures • New corrosion protective coatings and materials • Improve sensitivity of distributed analytical monitoring systems • Design and test under device working conditions of novel (cost/performance) competitive HTS nanostructured materials • Design of simplified generators using HTS and easy grid integration for high power wind mills. • Develop new coating to avoid corrosion and icing in the blades	• Incorporate automatic operation systems for de-icing. • Connect monitoring systems with integrated alarm procedures both for operational and environmental control. • Development of new low ac losses HTS conductors with improved quench resilience and cryogenic systems • Implementation of HTS devices for ultrafast electrical protection as HTS fault current limiters and SMES	• Development of new wind mill concepts and designs that outperform the current technology (e.g., sea movable structures, structures based in more than one tower, etc.) incorporating all the energy efficiency, aging and monitoring systems developed previously. • Incorporation of singular test facilities and pilot plants in collaboration with engineers and wind energy industry

	SHORT TERM (< 5 YEARS)	MID TERM (5-10 YEARS)	LONG TERM (> 10 YEARS)
GEOTHERMAL ENERGY	• Adaptation of the legislation to regulate the efficient use of geothermal resources • Development of techniques to efficiently enhance permeability of hot tight rock with a low risk of inducing seismicity • Successful demonstration of 5 MWe geothermal power plants in Enhanced Geothermal Systems (EGS)	• Achievement of high TRL for Organic Rankine Cycles (ORC) or kalina cycles to generate electricity at temperatures well below 100 °C • Development of reliable forecasting methodologies of induced seismicity • Scale-up of 5 MWe geothermal power plants in deep hot rock • Technological development of geothermal energy production in deep volcanic areas in pilot tests	• Generalization of the use of shallow geothermal resources to climatize buildings and district heating • Achievement of high TRL for the combination of geologic carbon storage with geothermal energy production at industrial scale • Widespread deployment of 5-30 MWe geothermal power plants in deep hot rock
FUSION	• Design and test under device working conditions of novel (cost/performance) competitive HTS nanostructured materials. • Development of computational tools to analyze HTS behavior on the device system. • Dedicated programs to strengthen joined collaborations between CSIC, institutions and industry.	• Investigation of the wire-to-device properties like thermal runaway, electromagnetic and mechanical properties, ac losses, electrical insulation, joints, geometries for compact fusion reactors	• Prof-of-concept for HTS tapes and magnets for the compact fusion concept

ONE SLIDE SUMMARY FOR EXPERTS

Challenge

Develop the knowledge and technology needed to substitute the use of contaminant power sources by clean and renewable ones.

Approach

The actual implementation of renewable energy as the primary source of energy in the world requires reaching the capability to provide energy in enough quantity, on demand and at a competitive price, just like conventional power sources currently do. The barriers towards this ultimate goal can only be overcome by improving the efficiency, stability, costs and manageability of the different clean technologies. These specific challenges have different mid and long-term implications for each one of the technologies considered, i.e. Photovoltaics, Concentrated Solar Power, Wind, Geothermal and Fusion.

Social and economic impact

There is an urgent environmental and economic need to substitute the traditional fossil based power sources, highly contaminant and main contributors to the greenhouse effect, for cleaner and renewable ones. This field will play a key role in the transition to a more sustainable economy worldwide. From a national perspective, it can be stated that our country is called to play a central role in the future development and commercialization of renewable energy. The existence of natural resources, a high level of technological advancement already achieved and the international recognition of our position in this field at all levels indicate that there is a clear opportunity to overcome the endemic and historical dependence of our economy on highly fluctuating activities such as tourism and construction and try to establish ourselves for the first time as world leader in a technology based market.

Involved teams

CSIC's research is aligned with European initiatives such as the EERA (European Energy Research Alliance). Its main strength lies in the high quality and wide diversity of expertise hold inside the institution, mainly, but not only, in the area of Energy Materials Science and Technology, with very relevant active public and industrial projects. Current activities target both the improvement of existing technologies and the development of new concepts and focus mostly in technology readiness levels (TRL) ranging from proof-of-concept to technology demonstration.

ONE SLIDE SUMMARY FOR THE GENERAL PUBLIC

Challenge

Develop the knowledge and technology needed to substitute the use of contaminant power sources by clean and renewable ones.

Approach

The actual implementation of renewable energy as the primary source of energy in the world requires reaching the capability to provide energy in enough quantity, on demand and at a competitive price, just like conventional power sources currently do. The barriers towards this ultimate goal can only be overcome by improving the efficiency, stability, costs and manageability of the different clean technologies. These specific challenges have different mid and long-term implications for each one of the technologies considered, namely, Photovoltaics, Concentrated Solar Power, Wind, Geothermal and Fusion.

Social and economic impact

Our world faces serious environmental and economic challenges. Climate change is directly linked to economic activity and specifically to the way in which we produce the energy we need. Thus, reducing the impact of human activity on the environment requires finding new cleaner ways of producing the energy we consume. For this reason, the development of stable, reliable, efficient and profitable renewable power sources is of outmost importance, now more than ever. Also, from a national perspective, this challenge poses an opportunity for our country to become a world leader in a technology based field in which we have already a strong position. This will help us overcome the endemic and historical dependence of our economy on low added value activities.

Involved teams

CSIC's research is aligned with all relevant national and international initiatives in renewable energy, and has a long tradition of productive cooperation with industrial partners working in this field. Current activities target both the improvement of existing technologies and the development of new concepts.

Hernán Míguez (Challenge Coordinator)

CHALLENGE 2

EFFICIENT ENERGY STORAGE

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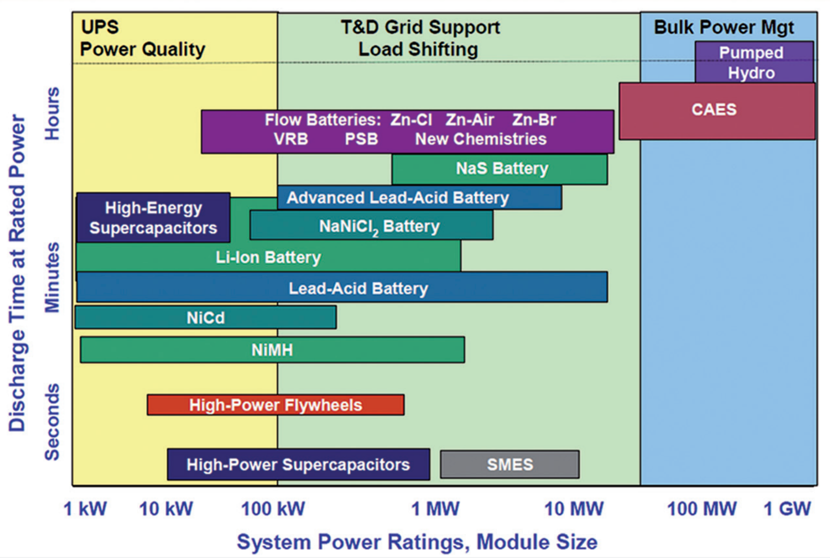
The deployment of energy storage technologies has not been considered a priority in the past because of their low relevance in a centralized fossil fuel energy landscape. Yet, the situation is evolving quickly as a result of the commitments to decarbonisation, which is in turn prompting improvements in cost for energy storage technologies. Transport electrification coupled to enhanced renewable energy penetration should bring about a drastic increase in the storage capability, especially considering the global increasing trend in energy consumption, not only in the emerging but also in the already developed countries. Moreover, storage is also crucial for introducing flexibility in the system and enabling distributed generation. At a European or Spanish scale, increasing storage should also enable a decrease in energy imports, yet, suitable regulatory frameworks are not yet fully established.

1. INTRODUCTION AND GENERAL DESCRIPTION

Energy storage technologies cover a wide spectrum of concepts,[Ibrahim] which can be classified according to different criteria, either purely technical such as permanent or portable, duration of storage (short/long term), amount of energy stored or power needed upon release or techno-economic such as maturity, efficiency, durability, cost, environmental impact etc. As a result of this diversity, energy storage technologies can match a wide range of specific applications (see Figure 1).

FIGURE 1–Characteristics of main energy storage technologies.[DOE]



A common classification, adopted by the European Association for Storage of Energy (EASE) and the EERA (European Energy Research Alliance) in their recently updated Energy Storage Technology Development Roadmap,[EERA 2017] bases on the storage principle and considers five families: (i) Chemical energy storage, which includes hydrogen as a vector, and is addressed in Challenge 8, (ii) Electrochemical energy storage (batteries, redox flow cells and supercapacitors, despite the later sometimes being featured under category (iii)), (iii) Electrical energy storage (SMEs), (iv) Mechanical energy storage (compressed air, flywheels, liquid air, pumped hydro) and (v) Thermal energy storage (sensible heat storage, latent heat storage, thermochemical heat storage).

Overall, a number of energy storage concepts already exist, some already having been around for decades. The current challenge is to achieve robust, reliable and economically competitive energy storage technologies, which would in addition, have to be matched to each specific application. The state-of-the-art, together with the current bottlenecks and CSIC position and potential evolution are described below.

2. ELECTROCHEMICAL STORAGE

2.1. Batteries

Batteries are chemical devices that store energy. They are made of two electrochemically active couples, the electrodes, typically solid, separated by an ion conductive, electronically insulating medium (electrolyte), commonly liquid. The electrochemical capacity (usually given in Ah/kg) of a given electrode material depends on the number of electrons exchanged and its formula weight while the voltage of the battery will depend on the difference between the potential of redox couples involved at each electrode. Battery performance depends both on the materials used at each electrode and cell design. While the former determine whether the system is rechargeable and has an influence on the range of possible operation conditions (temperatures, electrode kinetics etc), the later can greatly influence energy/power density balance, charging rate or cycle life. Secondary/rechargeable technologies are most relevant both in terms of size and value of the current energy storage market and future evolution perspectives. The three chemistries currently dominating the market are Pb/acid, Ni and Li-ion. Amongst these, the first two involve aqueous electrolytes (acidic and alkaline respectively) and have been "traditional" technologies which are now still being used in Starting Lightning and Ignition (SLI) for internal combustion vehicles (Pb/acid), Uninterrupted Power Supply (UPS) units (Pb/acid and Ni/Cd) or non plug-in hybrid vehicles (Ni/MH). Yet, their lower performance in terms of energy density, coupled to the toxicity of some components and to the decrease in cost of Li-ion technology have resulted in the latter progressively dominating the global market.

Indeed, Li-ion batteries enabled the revolution in portable electronics (Nobel Prize in Chemistry 2019) and are now the technology of choice for plug-in and electric vehicles while at the same time being considered for stationary grid applications.[Pillot] While the former comprise only one or a few cells, with energies being < 100 Wh, electric cars involve moving to the kWh scale, and hence assembly of battery modules and packs with a large number of cells controlled by the Battery Management System (BMS). Grid applications cover different scales and may reach the MWh. The share of the three applications are expected to represent 15%, 80% and 5% of the total global battery market in 2025 respectively, with a global growth in the next 10-15 years driven by the irreversible move towards transport electrification.

Impact in basic science panorama and potential applications

Lithium-ion batteries operate through reversible (and usually topotactic) insertion of lithium ions in the electrode materials structure. In practical cells, electrodes are conventionally tape casted on a metal current collector (aluminium for the positive and copper for the negative), and aside the active materials contain additives to enhance electronic conductivity and a binder to improve adhesion, mechanical strength, and ease of processing. Positive and negative electrodes are separated by a microporous film, and the whole assembly is impregnated with the electrolyte. Common electrolyte solvents (linear and cyclic alkylcarbonates) are unstable below ca. 0.8V vs. Li^+/Li and above ca. 4.5V vs. Li^+/Li in contact with electrode materials, which are strongly reducing/oxidizing. The resulting insoluble products form a solid protective passivation layer adhered at the surface of the negative electrode, (termed the Solid Electrolyte Interphase, SEI) which enables operation of the electrolytes outside their thermodynamic stability windows. Despite a large spectrum of materials being investigated at the laboratory or pre-commercial scale,[Croguennec] the diversity of compounds used in commercial cells is rather low. These are typically graphite at the negative electrode (despite $Li_4Ti_5O_{12}$ being also used sometimes) and layered transition metal oxides ($LiMO_2$ with M mostly corresponding to Co or a mixture of Ni, Co and Mn or Ni, Co and Al, typically termed NMC or NCA respectively), $LiMn_2O_4$ or $LiFePO_4$ at the positive. Performance has been gradually improving as a result of both improvements in materials and also cell design, involving also non active materials (current collector, separator).[Placke, Blomgren]

European stakeholders have defined a scheme on current and future generations of Li-ion technologies to be developed basing on the materials involved.[EMIRI] It starts with Generation 1, which consists of the commercial technologies mentioned above and Generation 2 involving the use of NMC ($LiNi_{1-x-y}Mn_xCo_yO_2$, commonly denoted NMC111, NMC523 with figures representing the relative ratios of Ni, Mn and Co), with enhanced nickel content, which provides higher capacity despite lower cyclability, already being commercial now. Generation 3 represents the short-term prospects (< 5 years) currently at pre-commercial stage which, besides further increase in nickel (and concomitant decrease in cobalt) in NMC (NMC622 or NMC811), involves addition of a significant percent of silicon to the graphite negative electrode to enhance capacity and hence energy density. Indeed, materials with a redox mechanism not based on topotactic insertion but on electrochemical alloying enable much higher capacities due to the fact that they react with a larger amount of Li ions, such as Si, which can electrochemically form $Li_{15}Si_4$ and has also the advantages of abundance and low cost. Yet, this comes to the expense of significant high volume change at each charge/discharge half cycle which ultimately lead to poor cycle life, and despite widespread intense efforts worldwide basing on a myridad of approaches, only electrodes with few percents of silicon meet the cyclability criteria for practical application. Beyond the above mentioned generations, alternatives considered within a longer timeframe are Generation 4, using solid state electrolytes (either polymer or inorganic) and Generation 5 (beyond Li-ion), focusing not only on the use of lithium metal as negative electrode but also on new technologies which should also be able to enable high energy density and based on abundant materials with low cost.

Key challenging points

The boost of the consumer electronics market has triggered continuous research driven improvement in the energy density for Li-ion batteries. Yet, larger scale applications such as transport or grid, require different priorities in the consideration of the figures of merit in terms of energy, power, safety, durability, cost, sustainability etc. An as an example United States Advanced Battery Council (USABC) goals involve extension of battery life to 15 years for transport applications considering a wide temperature operation range (-30 to 52°C). In addition to enhanced lifetime (which contributes to decrease the life service cost), both grid and transportation impose more stringent requirements in terms of cost, safety and sustainability (e.g. CO_2 footprint, recycling etc.). Challenges ahead for the Li-ion technology are outlined below:

Electrodes: Materials enabling higher energy density at cell level while keeping good cycle life should gradually be implemented. On the positive side this involves developing reduced (or null) cobalt content layered $LiMO_2$, with decreasing cobalt content resulting also in a decrease in cost or else considering also either the so-called Li-rich materials (x $LiMO_2$·1-x Li_2MnO_3), or the $LiNi_{0.5}Mn_{1.5}O_4$ spinel, none of them containing cobalt, but still suffering from limited cycle life. On the negative case, the quest should focus on electrodes with higher percent of silicon (or SiO_x). Beyond the material level, processing protocols do also deserve attention, as fabrication of casted electrodes from water-based slurries instead of toxic organic solvents would bring in decreased cost and enhanced sustainability. Yet, given the aim for very high operation potential on the positive side, reactivity with moisture remains a concern to address.

Electrolyte: The composition of the electrolyte faces stringent technological requirements, and $LiPF_6$ based formulations are the only compliant option to date, with corrosion of Al current collectors being the main bottleneck for the implementation of new salts. In order to enhance energy density (e.g. high cell operation voltages) while keeping safety and cycle life, the use of electrolyte additives seems to be the only promising approach, despite the complexity of the research involved, still entailing a lot of emprisim.[Burns]

In the case of lower TRL technologies, more fundamental challenges apply:

All solid state batteries: While at the materials level the development of electrolytes with high ionic conductivity and large stability window is a must, processing of materials involves and added complexity especially for inorganic electrolytes (either glass or crystalline). Cell manufacturing is not trivial either, and mastering of the processes to achieve high quality solid/solid interfaces are a must. In case of concepts using lithium metal anodes, dendritic growth and volume change during charge/discharge steps are supplementary issues to solve/manage.

Beyond Li-ion chemistries: while practical development Li metal based concepts (Li/S or Li/air) involve both mastering the reactivity of Li, the former suffers from a too low amount of sulfur in electrodes with good performance, while for the later the development of suitable air electrodes with bi-functional catalysts and the fundamental understanding of the redox mechanism are still major roadblocks. Non lithium based chemistries may exhibit significant advantages in terms of cost and sustainability if suitable components are developed. For the case of Na-ion, fast progress is expected as a result of the *know how* available in the Li-ion field. Cells are unlikely to outperform Li-ion in terms of energy density, major projected advantages being in cost and sustainability. In order to achieve high energy density the use of metal anodes seems compulsory, with multivalent metals (Mg, Ca and Al) being attractive alternatives. Given the very low current TRL of such concepts, suitable standards and protocols/methodologies need to be developed and hence require essentially fundamental research.

All these challenges call for expertise in materials science and engineering, covering not only experimental but also modelling aspects, with also some contribution from electronics (battery management systems) and modelling coupled to artificial intelligence to guide materials discovery. These can contribute to both high TRL research (expected to be mostly industry-driven) but most specifically to low TRLs aspects involving new technologies and tools/methodologies for characterization not only of materials but also of processes taking place *operando*, in cooperation with large research infrastructures when needed. The outcome should be full comprehension of safety and degradation mechanisms, with improved understanding of interfaces/interphases, progress in eco-friendly low-cost materials and electrode processing and recycling protocols, and development of new high energy density low cost technologies avoiding the use of critical materials.

2.2. Redox Flow cells

Impact in basic science panorama and potential applications

Redox Flow Batteries (RFB) are one of the more promising energy storage technologies for grid applications related to integration of renewables (wind, photovoltaics) at large scale, in the order of MW / MWh. Their most interesting features are their flexibility, as the geographical restrictions related to mechanical concepts do not apply, and their decoupling of energy and power enables them to be designed independently. Power depends on the size of the electrochemical "stack" where the oxidation-reduction reactions take place, while energy depends on the electrolytes (their nature, volume and concentration). The electrochemical system is made up of two electrodes (or a stack of electrodes) usually made of carbon materials. Electrodes are not the active materials where energy accumulates, as in classic batteries such as lead-acid or lithium-ion. In this type of batteries, the electrodes are not modified but they act as electrocatalytic surfaces on which the oxidation-reduction reactions of the electrolyte occur. In redox flow batteries there are two electrolytes separated by a membrane. Each electrolyte undergoes its own oxidation-reduction processes during cell loading and unloading. How fast the electrolytes are transformed onto the carbon surfaces determines the power of the system that depends mainly on the efficiency of the electrochemical cells, and the size and number of stacks. The fluidodymamic of the system, which maximizes the contact of the electrode surface with the flowing electrolyte, is also a key parameter for the performance of the battery.

The electrolytes are not only contained within the electrochemical system, as in the case of most conventional batteries, but are stored in two separate tanks, one for the positive electrolyte, and one for the negative electrolyte. From these tanks they are pumped into the electrochemical cell (this is why they are called flow batteries), where they are transformed and returned to the tank. As long as there is electrolyte that can be transformed, the battery can continue to charge (or discharge). This is why the energy that can be stored depends on the volume of the tanks, the more electrolyte the greater the energy that will be stored. More precisely, it depends not only on the size of the tanks, but also on the concentration of the electrolyte and its chemical nature.

The more developed flow batteries are the All-Vanadium Redox Flow Batteries (VRFB) [Zhang] where both electrolytes are made up with vanadium salts. The positive one uses VO^{2+}/VO_2^{+} sulphates in sulphuric acid solution, with approximately 2M concentrations. On the other hand, the negative electrolyte uses V^{2+}/V^{3+} sulphates also in sulphuric acid with analogous concentration. Recently some improvements have been achieved using HCl acid mixed with H_2SO_4 to increase solubility and stability of vanadium salts.

Key challenging points

The challenges of building a battery comprise two key aspects that are better understood when the battery structure is known. One is the chemical or electrochemical part, where the different components of the battery play an essential role. The second aspect has to do with the engineering design of the cell, taking into account critical aspects such as the fluid dynamics of the electrolytes, and the assembly, sealing and instrumental control of the cell.

Some comments on the key components are given below.

Electrolytes: A suitable electrolyte requires a high concentration of active species (to increase the energy density of the battery), high stability within the working potentials and thermal stability (-5 to +50 ºC). Although different pairs of electrolytes (such as Iron / Chromium or Zinc/Bromine) have been tested over the years, there is no doubt that vanadium electrolytes have been the most successful ones. In order to improve the results obtained for vanadium solutions many different additives have been used, the best results obtained up-to-date being with the use of mixed H_2SO_4-HCl solutions that allow high concentrations of vanadium salts (up to 2.7 M) and are stable in a wide range of temperatures (-5 to + 50 ºC). Extraordinary efforts are being made in the development of new organic electrolytes [Winsberg, Leung] that can substitute inorganic ones as they always present some limitations (as unstable cost and limited resources in the case of vanadium). The main limitation of organic electrolytes is found in the stability of the redox couples and the difficulties in the synthesis of compounds that present high potentials.

Electrodes: Many different materials have been tested as positive or negative electrodes in RFB.[Zhang] They can be grouped in two categories, metals and carbon materials, with consensus carbon materials being preferred. Amongst these, carbon fibre felts are the most relevant due to their relatively low cost, easiness of handling and electrochemical stability. However commercial carbon felts show poor performance and modifications are normally performed. Oxidising the carbon surface (chemically, thermally or electrochemically) is an easy way to improve performance. Nevertheless, many efforts are devoted to increase electrocatalytic activity of carbon surfaces and the addition of chemical species (carbonaceous or not) is a major issue on the research of positive and negative carbon electrodes.

Membranes: they are a key element in RFB and ideally need to combine different properties.[Prifti] High ionic conductivity is compulsory for charge transport in order to maintain the electroneutrality of the two half cells, yielding a low electric resistance per area. At the same time, low permeation rates for water and the redox active species (vanadium ions) are also needed. In addition to those, chemical and mechanical stability are also required for good cycling performance during the battery life. No doubt that Nafion membranes fabricated by Dupont (cationic membranes with excellent proton transportation properties) are the most widely used RFB membranes in spite of their high cost. Nevertheless, research is focussed in improving membrane selectivity by adding inorganic particles, surfactants, etc. New types of membranes are under research, especially anionic membranes that present very low permeation for vanadium species, but unfortunately ionic transport is rather poor compared to nafion membranes.

Fluidodynamics: The structure of the flow field of the electrolyte within the electrodes determines several parameters that have a deep impact on some critical features of the stack, such as the mass transfer rate of the electrolyte, current distribution, overpotential distribution, etc. Therefore, the overall performance of the cell greatly depends on the design of the flow channels that maximizes the electrode-electrolyte contact.

Engineering: The materials selected and the final construction of the cell also play a critical role in its operation and cost.[Noack] Avoiding both internal and external leaks improves performance, safety, and cell durability. Proper mounting of the stack also helps to maximize voltammetric and energy efficiency, reducing energy consumption in the pumps and the electrical resistance of the assembly. The determination of the state of charge of the cell is a very important issue that is still not fully solved. Another important questions to be considered in large flow cells is the heat management to maintain the electrolytes temperature within the required range. Finally, electronic control of the cell also plays an important role in the final output performance of the stack and in the safe use of it.

2.3. Supercapacitors

Supercapacitors (SC)[Wang, Proonam] are devices for storing electrical energy that fill the gap between electrolytic capacitors and batteries. The output power of supercapacitors is less than that of electrolytic capacitors, but their specific energy is several orders of magnitude higher. On the other hand, SC are capable of providing high power rates compared to batteries, although their capacity to store energy is much more limited.

Current supercapacitors display energy densities of 5-10 Wh/kg, while supplying power pulses above 10 kW/kg. Additionally, these systems present an operating life over 10^6 charge-discharge cycles, excellent operation in a wide range of temperatures and easy maintenance. They operate efficiently during short times (< 1 s to 90 s) and are successfully applied in urban transports (bus, tram and train), industrial vehicles (excavators, cranes, forklifts) and stationary systems (grid and uninterruptible power supplies). They are also part of electronic devices such as computers, telephones, wireless tools, traffic signals, etc. The smallest niches for SC are the aerospace, military, and medical industries. Market studies converge towards revenues of around 1,500-2,000 M€ for 2022.[Schutter] A growth rate higher than 25%-year is expected due to the needs for recharging the batteries of hybrid vehicles or starting electric vehicles. In this context, Tesla has just bought Maxwell Technologies, the number one producer of supercapacitors worldwide.

Impact in basic science panorama and potential applications

Briefly, a supercapacitor is made of two electrodes with a separator between them, which are soaked in an electrolyte. Based on the operating mechanism, these devices are divided into Electrochemical Double-Layer Capacitors (EDLC), Pseudocapacitors and Hybrid Capacitors.[Wang, Poonam] The majority of commercial supercapacitors are EDLC that operate by the electroadsorption of electrolyte ions on the surface of activated carbons, without Faradaic processes. Pseudocapacitors perform by fast and reversible charge transfers at the surface of electroactive materials (i.e. transition metal oxides and conducting polymers) or involving redox reactions of the electrolyte components. The combination of both EDLC and pesudocapacitive processes results in hybrid capacitors. Attending to the cell configuration, the electrodes in asymmetric SC differ in charge storage mechanism, composition or weight, while they are identical in the symmetric devices.[Shao] Supercapacitors can operate with liquid or solid/quasi-solid-state electrolytes.[Wang, Schutter] Actually, most commercial SCs use organic electrolytes such as Et_4NBF_4/acetonitrile, since they allow reaching higher operating voltages than aqueous solutions. High power density, long service life and low cost in terms of €/kW of actual supercapacitors meet the requirements for most applications, but their low energy density or rather their high costs in terms of €/kWh are the main barriers for large-scale implementation. [Schutter]

Key challenging points

At the present, there are basically two strategies in the supercapacitors market. One of them is devoted to achieve much higher energy density and the other is looking for a comparable performance but at a much lower cost.

Additionally, there are numerous challenges for Next Generation-Supercapacitors both for those targeted for high-power applications on the grid (to smoothen the leftover alternating current ripples and to harvest electrical energy from low-grade heat sources and renewable energy) and for multifunctional supercapacitors (micro-SC, self-charging SC, self-healing SC, flexible-stretchable-compressible SC, bio-compatible/-degradable SC, etc.) to consumer electronics.[Wang, Poonam]

In this context, RD&I efforts are primarily devoted to the following issues: [Wang, Poonam, Schutter, Shao]

Novel electrode materials. The search is currently directed towards better performance/cost ratio and focuses in:

Active materials. Among others, graphene-type materials, nanotemplated carbons, CNT films, MOF, COF, MXenes, black phosphorus, low-cost metal oxides (MnO_2, CO_2O_3, NiO, SnO_2) and mixed oxides ($LaMnO_3$, $SrRuO_3$), MoS_2, VN, electroactive polymers (PPy, PEDOT, PANi, PTh) and composites made from the combination of the above are being studied in depth.

Conducting agents. A small amount of graphite or carbon black is generally added to increase the electrical conductivity of the electrode. Other more advanced carbons (CNT, graphene, etc.) provide better performance but their price is still too high.

Binders. New products are required to increase loading of active material, while retaining electrode integrity for long operating cycles. In addition, they must have lower density and cost and better recycling than the standard PTFE and PVdF currently used.

Electrode processing. Besides the industrial production of stable electrodes with the highest amount of active material, the minituarization and flexibility are also being regarded as key challenges for the most sophisticated applications.

Advanced electrolytes. Extensive efforts are being devoted to explore new electrolytes and solvents that enable operative voltages higher than 3 V and display lower viscosity and higher conductivity. Additionally, toxicity, melting point, boiling point, and flash point determine the safety and the temperature range of the final device.

At the present, ionic liquids and electrolytes enriched in solvated redox-active species appear as promising strategies, whereas solid-state or quasi-solid-state media are an option for all-solid-state and flexible devices.

Separator. It must be ion-permeable and, simultaneously, have a high electrical resistance and low thickness. A number of materials based on glass fibers, ceramics, and advanced polymers are already under investigation as substitutes for the standard ones (cellulose or polypropylene).

Novel device designs. Asymmetric capacitors and those with a hybrid configuration offer great apportunities and are being extensively studied. *Supercapattery* is a recent term proposed to describe a wide variety of devices in which the charge storage mechanisms are combined to reach the high power of SC and the energy density of battery.[Wang, Poonam]

Nanoscience for advanced electrodes and devices. Wearable electronics and advanced aerospatial and medical applications focus the priority in multifunctional supercapacitors with a number of capabilities, such as minituarization, flexibility, transparency, and ability for self-charging/-healing/-repairing, etc.[Poonam]

Low TRLs also need standard testing protocols, advanced *in situ* characterization techniques and theoretical studies and *ab initio* simulations of the SCs mechanisms.

3. OTHER TYPES OF STORAGE

3.1. Thermal

Impact in basic science panorama and potential applications

Thermal Energy Storage (TES) is able to achieve massive energy storage capability in the foreseeable future.[Alva, Carrillo] Solar energy is an example of successful integration of energy production with TES as most Concentrating Solar Plants (CSP) currently under construction or planning stages incorporate some sort of TES system.[Fernandez] Nevertheless, such systems could be integrated into any other renewable energy technologies by converting electricity surplus into stored heat. TES systems are classified into three main groups; sensible heat storage (SHS), latent heat storage (LHS) and thermochemical energy storage (TCES). All TES systems are based on the heat absorption and heat release processes by the storage media during charge and discharge cycles.[Zhang2016] Sensible heat storage (SHS) systems exploit the raises and drops in temperature of the storage media: water/steam, solid particles, oils, solid and liquid metals and the state-of-the-art high temperature storage in inorganic salts ("solar salt").[Weinstein, Kuravi] Current strategies to improve energy storage density and heat losses comprise the synthesis of composites, nanofluids or eutectic mixtures.[Vignarooban] Latent heat storage (LHS) systems rely on the heat absorbed or released by the storage media during a phase change. LHS systems encompass organic compounds such as paraffin and fatty acids, inorganic materials such as salt hydrates and metal alloys and eutectic materials (either organic or inorganic).[Pielichowska] Phase segregation, subcooling or heat losses during storage constitute a significant problems. Currently, microencapsulation of materials is attracting a lot of attention as a method to contain phase change materials (PCMs) while increasing the heat transfer surface area; prototypes have been constructed in projects carried out by the German Aerospace center or by the Sunshot Initiative from the U.S. department of Energy USA.[Xu] Finally, thermochemical energy storage (TCES) is the least technically developed system, but with large theoretical energy densities, surpassing even that of Li-ion batteries. In the last years, a number of large projects have been started all over the world to explore the potential of this storage system such as the Sunshot Initiative.[SunShot] Most studied TCES systems include ammonia, sulfur-based, metal hydrides, carbonates, hydroxides, hydrocarbons, redox reactions and sorption processes.[Zhang2020]

Key challenging points

As recognized by the European Energy Research Alliance, TES technologies can be highly beneficial to a variety of applications; increasing energy efficiency in industrial processes and buildings, integration of low carbon energy for heat generation and to improve district heating and cooling performances. [EERA 2017] However, only SHS and low scale and room temperature LHS have actually reached technological maturity and commercially availability. There is a great interest in high temperature PCMs combining both sensible and latent storage. Moreover, whereas TCES systems offer the highest theoretical energy densities, most are still in very early stages of development so that very important resources need to be devoted in the next years to cover the gap between research aspects and system aspects.

The main objectives and research priorities to pursue in the following years within this field can be summarized as follows:

- Develop new Sensible and Latent heat storage media and Heat Transfer Fluids with enhanced properties (improved heat capacity and thermal conductivity, extended range of operation, long term reliability) by using nanofluids, new compounds, composites, encapsulation, etc.
- Identification of TCES systems with high energy density and feasible application at large scale. Attain full control of reaction requiring deep understanding of thermodynamics, kinetics and modelization. New reactor concepts.
- Design of advanced materials for high temperatures and highly corrosive environments compatible with TES applications: ceramics or cermets, coatings, corrosion inhibitors, etc.
- Devise reliable testing and characterization techniques for *in-situ* measurements at working conditions (high temperatures, high flows, high pressures, etc)
- Integration of high temerature storage into diverse processes such as renewable energy technologies, different from CSP, by converting electricity surplus into stored heat or space heating in buildings

3.2. Mechanical Energy Storage

Key challenging points

Among the large portfolio of different proposals for energy storage[EERA] mechanical devices have been considered from the early times, given advantages in independence between power and amount of energy stored. The basic technology is well understood and exhibits good efficiency and large life time. Strictly mechanical systems use gravitational or mechanical elastic energy and can store large amounts of energy as is the case of Hydropower plants used for leveling the demand of energy improving the regulation capacity of the grid. Other alternatives are compressed and liquefied gases performing open or closed thermodynamic cycles. These enable storing energy in large amounts including heat exchange (hybridation with thermal energy storage). CAES (Compressed Air Energy Storage) uses thermal sources for compensating the cooling of the air in the expansion section of the cycle [Luo] and ACAES (adiabatic version of CAES) which stores heat during the compression have been demonstrated with good efficiency (around 70%).[Biasca] Other options involve expansion of liquefied cryogenic gases as is the case of Liquid Air Energy Storage (LAES). Liquified air is produced in the charging process and expanded in a turbine using residual waste heat from industrial processes including cooling systems, recycling plants and others.[EERA2017] Open Cycle conception where LA is produced in liquefying plants and distributed as fuel to cars and trucks is also possible.[Dearman] Mechanical kinetic energy has been also exploited as energy storage system and essentially consists of a rotating flywheel activated by an electrical motor-generator which allows transforming kinetic energy to electricity. Its amount depends on both, the rotation speed and the inertia momentum. The former is limited by mechanical concerns. The energy stored cannot be absolutely exchanged because the generator rotational requirements and limited to ca. 75% of the full energy stored in the wheel.

Flywheels are installed as emergency energy suppliers and allowing a very fast intervention being able to supply power in milliseconds. The efficiency is in the range of 90% with a high robustness that allows overcrossing the nominal power threshold without degradation. There are several manufacturers of steel based flywheels ranging from kW to MW.[Alba]

Current challenges in mechanical energy require research in materials science and also in electronics concerning materials with specific thermal properties able to efficiently store the heat delivered in the compression (ACAES). In that case, mechanical storage requieres also thermal storage to be efficient. Heat could be stored but also can be harvested from external sources as the so called heat waste. Low temperatures can be achieved with the use of liquid cryogenic gases. Experiments in are an oportunity for diminishing the medium level cryogenics cost via systems to be used between 77K to 110K as rejection temperature for cryocoolers. Flywheels for Energy Storage offer opportunities for research by developing new light materials with large yield stress such as composites based in carbon and silica fibers, nanotubes and graphene based materials. These enable a better equilibrium when deformed by the centrifugal stress, enhancing the possible rotation speed. Bearings are a critical point. They should support very high loads in a permanent actuation. In the present state of the art, the bearing load is compensated by contact less magnetic actuators that can be substituted by frictionless noncontact Superconducting levitators enabling high rotational speeds.[Strassik] Full Superconducting Flywheels allow improving the energy density with lighter systems with lower mass, inertia and kinetic moment: a step forward to the possible extension to mobile systems

3.3. Electromagnetic Energy Storage

The Faraday-Lenz Induction law shows that electrical field and magnetic field have temporal dependence: The change of the magnetic flux trough an electrical circuit creates an alectrical current. This effect refers to magnetic field independently of how it is produced. It is well known that a current in a circuit induces a magnetic field and so a magnetic flux crossing the circuit is created, which is known as selfinduction. Any change of the electrical current in a circuit means an extra electromotive force where the selfinductance, represents the ratio between the magnetic flux and the electrical current producing that flux. Any change in the current in a circuit produces a voltage as larger as faster is the change of the current. Since the early times of electromagnetism, this phenomenon, has been extensively used in filters, transformers and oscillators among a large set of devices and applications. The energy associated to a magnetic field depends on its density and the volume of field. In order to have an idea about the amount of energy stored in the coil producing the field, we can compare it with the gravitational energy: the energy corresponding to a cubic meter of magnetic field with a density of 1T is equivalent to the energy of 1 cubic meter of water at a high of 40.6m. However, the capacity of coils to store energy in large amounts has not been exploited until the discovery of superconducting materials because in a closed circuit the magnetic field decays in a very short time due to the electrical resistance, losing energy as heat. Superconductors are able to carry the large amount of electrical current needed to produce the magnetic field with densities in the range of several Tesla. The first official proposal was around 1970. [Ferrier] before the discovery of the High Temperature Superconductors (HTS), and led to the construction of the first SMES System installed in the electrical grid of Boneville Power Authority by 1980.[Boenig] A series of SMES based in the standard superconducting cabling were developed at the starting of the XXI century enabled by the development of the required technologies. One of them was developed in Spain (1MJ-500kW project Amas 500). [Bautista]

Key challenging points

The discovery of the so called High Temperature Superconductors introduced a new qualitative step and also new challenges associated to the characteristics of the new materials that had demonstrated the possibility to achieve very high magnetic fields such as 45.5 T at Tallahassee magnetic facilities. The differences introduced affect the coil manufacturing, the cryogenics and the control systems. The difference between the cables manufactured with the old Low Temperature Superconductors (LTS) is established essentially by the ceramic nature of the HTS that does not allow the manufacturing of ductile wires. In order to get the necessary bending for the coils processes have been developed to create superconducting thin coating over metallic substrates, the so called Coated Conductors. The bi-axially textured ceramic HTS coating allow flexibility to perform the windings and can withstand very high current densities at high field, able to work efficiently at temperatures in the range of 20K to 40K. It simplifies the cryogenics and improves the efficiency at the same time enabling the achievement of a large field. Although there are about 7 companies in the world that sell the HTS wires, a huge effort is running to reduce costs to make it competitive in front of other storage technologies. The most relevant benefits of SMES systems are:

- **Efficiency** in the range of 90 - 97%. (including energy needed to keep cool the system)
- **Long life,** estimated in 30 years, with maintenance essentially associated to the cryogenic cooler. Nowadays it is required every 20,000 - 30,000 hours but new free piston machines allow useful life beyond 200,000 hours without maintenance.
- **Charge and discharge power** is essentially defined by the electronics, the electrical isolation and the cooling margin of the cryo-system,
- **Readiness:** Can deliver its peak power in the millisecond range.
- **Robustness**. There is no degradation by cycling and some SMES have been working from more than 15 years without degradation
- **Hybridization**. The system allows working within the buffer electronics that allows connection between practically any power source allowing filtering the power transients which damage other energy sources.

- **Mobility**. Although deformations in the coil could represent changes in the magnetic flux, safe mobility of the SMES with possibility to be installed in transporting devices can be envisaged.
- **Low environmental impact** along its lifecycle: most components are recyclable, contain very low amounts of Rare Earths, if any. Closed magnetic circuits are feasible which exhibit very low magnetic impact.

The cost of the SMES is essentially due to the cost of manufacturing the biaxially textured coatings, which means a single-crystal-like structure of kilometers long. This structure should have a nano-structure of defects which allow trapping the magnetic field quanta wrapped by the paired electrons which conform the so called vortex. The pining of such vortex allows fixing the magnetic flux lines and avoids their displacement due to the electromagnetic forces when current is flowing through the superconductor. Conducting without energy losses needs fixing the vortex lattice. The maximum magnetic field supported and the maximum critical current are strongly related with the nanostructure of defects. A great effort is being done in this sense by specific engineering of the coatings. Quality at a good price diminishes the cost in two ways: the cryogenics could be simpler and the length of wire can be shorter.

The cost of the material is also related to the production and the cost of development payback. Although manufacturers start to be abundant, at the moment the demand is low and no stable production exists, Lower cost and faster coating manufacturing would diminish the effective cost to prices equivalent to copper or even lower. Materials are good, although there is still room for improvement (larger magnetic field, lower AC loses, better joints, better mechanics, improved quench resilience). Fusion needs a large amount of these materials. They allow an step forward in the design of tokamaks to the so called compact tokamaks in which the size is substantially diminished by increasing the confinement magnetic field.

Hybridization is the concept in which the roadmaps for SMES make more emphasis. In fact, batteries, mechanical storage as LAES, ACAES etc, can get benefit of the robustness and readiness and the high power capacity of the system. In some cases Hybridizaation allows Symbiosis as is the case of Liquid Air Energy Storage (LAES). The optimization of the role of SMES and its coordination with the improved long term energy storage systems is a topic of research for static grid applications and there are some proposals for mobile systems linked to transport.

Cryogenics is at the moment linked to research from small labs, including satellites, to very large installations for accelerators and fusion. However compact systems for medium scale fulfilling the requirements of large market applications are systems not developed enough. A simple robust and efficient system is needed. Systems based on Helium working at 20K could improve efficiency using hydrogen, lighter than helium and with larger thermal capacity. In summary there are research needs concerning the materials, (structural, isolators, superconductors, thermal conductors), cryogenics, hybridization, and symbiotic systems.

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TABLE 1–List of challenges to be addressed for the Challenge 2

TECHNOLOGY		SHORT TERM (<5 YEARS)	MID TERM (5-10 YEARS)	LONG TERM (10-20 YEARS)
ELECTROCHEMICAL STORAGE	**Batteries**	• Enhance energy density while keeping cycle life via optimizing: - High Ni content NMC or high voltage positive electrode materials - High Ni content NMC or high voltage positive electrode materials - Si based negative electrode materials • Electrolyte formulation/additives • Study of ageing mechanisms covering all battery components • Development of sustainable electrode processing protocols	• Achievement of high TRL for sustainable low-cost efficient Na-ion technologies. • Achievement of high TRL for all solid state batteries with Li metal anodes, including suitable manufacturing protocols. • Development of low-cost sustainable recycling processes covering a wide range of specific chemistries/ materials.	• Proof-of-concept for high cyclability and high energy density concepts with metal anodes: - Li based (Li/S, Li/ O_2) - Multivalent chemistries (Zn, Mg, Ca, Al)
	Redox flow cells	• Development of 10kW stack based in vanadium electrolyte. • Achievement of higher current densities than state of the art cells.	• Development of new organic electrolytes and suitable electrodes and membranes for them. • Involvement of industrial sector for scaling up the technology	• The technology arrives to full commercial scale
	Supercapacitors	• Increase electric storage capacity by 50% and/or significantly reduce SCs cost by: • Novel electrode components and electrolytes • New configurations tailored to market demands. Safety and LCA • Sustainable electrodes processing and SCs set-up • Join industrial clusters involved in energy transition	• Design and manufacture prototypes (cells and modules) for strategic markets. Operation validated by DEMOs and test-bench • Assessment of techno-economic perspectives targeting diverse niche markets. • Roadmap for sustainable and profitable SCs production. Synergy with other EES	• Scale-up and standardization of novel SCs production. Cutting down technology costs. • Business cases: Market uptake of the new developments and technology

TECHNOLOGY		SHORT TERM (<5 YEARS)	MID TERM (5-10 YEARS)	LONG TERM (10-20 YEARS)
THERMAL STORAGE		• Improvement in cyclability and high thermal energy density (composites, mixtures, additives, change in composition, encapsulation, etc) at lab and prototype scales. • Improvements in thermal properties (enthalpy, Cp, thermal conductivity, thermal stability) to achieve higher efficiencies	• Achievement of high TRL for integration of high temperature thermochemical energy storage within CSP plants • Development of hybrid TES based on the use of several combined systems (sensible, latent and thermochemical heat storage) for broader temperature ranges.	• Integration of thermal energy storage with other technologies and industries • Use of thermal energy storage for non-thermal renewable energy sources (PV, wind turbines) • Large scale storage
MECHANICAL STORAGE	**LAES & ACAES**	• Developement of heat Storage means for 200°C and capacity to transfer the heat by regeneration of heat exchangers • Design of turbines with multy stage with inter-stage heat rejection-cooling • New systems adiabatic&isobaric • Viability studies for liquid CO_2	• Developement of Hybrid systems SMES-LAES for industrial Parks • Improving the distribution network of cryogens as Liquid Air • ACAES for Local Storage of energy (PV and Wind) • LAES for transport developments	• Developement of Hybrid systems SMES-LAES for industrial Parks • Improving the distribution Network and the LA resources
	Flywheel	• Improvement of composites for achieving high mechanical strengh wit low densty materials • Improvement of high homogeneity precisión manufacturing of flywheels • Low density very high strength materials	• Low cost HTS materials for levitation • High stability HTS bearings • Cryogenics in flywheel systems • Introduction of full HTS flywheel	• HTS Ultra High speed Wheels • Flywheels in transport

TECHNOLOGY	SHORT TERM (<5 YEARS)	MID TERM (5-10 YEARS)	LONG TERM (10-20 YEARS)
MAGNETIC STORAGE	• Development of lower cost HTS tapes for working at 8T • Development of modular concept for manufacturing of coils achieving lower manufacturing costs • Improvement of the early detection of quench • HTS SMES enters in the electrical grid	• Development of lower cost HTS tapes for working at 12T • Development of medium level heat rejection cryo-systems for Hybrid applications LAES-SMES, LNG-SMES for industrial Parks • Development of HTS conductors with very low AC losses • HTS enter in more electric aircraft	• Liquid Hydrogen symbiotic + Hybrid Energy Storage systems • SMES for Energy recovering and power boostering in Transport • HTS enter in standard FACS systems for smart grids

ONE SLIDE SUMMARY FOR EXPERTS

Challenge

Provide the knowledge and technologies required to significantly increase the amount of energy stored, which currently represents a tiny fraction of the total amount of energy generated and consumed worldwide.

Approach

Energy storage technologies are rooted in different storage principles (chemical, electrochemical, thermal, electrical, mechanical...) and enable a wide diversity of concepts delivering different performance in terms of amount of energy stored, duration, efficiency, portability, etc. Amongst these, electrochemical energy storage (batteries, redox flow cells and supercapacitors) are the focus of intense research efforts, given their versatility and wide spectrum of applications. Other concepts such as thermal, mechanical or electrical energy storage are complementary and are being used in more specific scenarios. Additional requirements beyond technical figures-of-merit are affordable cost, sustainability and low environmental footprint.

Social and economic impact

Enhancing energy storage would enable flexibility to deliver energy *when* and *where* it is needed and to decouple generation from consumption. The main societal impact is related to the electric grid, as storage would allow maximizing the percent of renewable energies integrated. Some portable storage technologies, such as batteries, fulfil the technical requirements to power vehicles and have the potential to trigger electrification of transport, which would also greatly influence our current way of life. Both transformations would result in a drastic decrease in fossil fuel consumption and hence significantly reduce CO_2 emissions paving the way towards a greener energy landscape.

Involved teams

CSIC's research is aligned with European initiatives such as the EERA (European Energy Research Alliance) and its main strength is rooted in the Materials Science expertise. Current activities target both the improvement of existing technologies and the development of new concepts and focus mostly in technology readiness levels (TRL) ranging from proof-of-concept to technology demonstration.

M. Rosa Palacín (Challenge Coordinator)

ONE SLIDE SUMMARY FOR THE GENERAL PUBLIC

Challenge
Provide the knowledge and technologies required to significantly increase the amount of energy stored, which currently represents a tiny fraction of the total amount of energy generated and consumed worldwide.

Approach
Energy storage technologies are rooted in different storage principles (chemical, electrochemical, thermal, electrical, mechanical...) and enable a wide diversity of concepts delivering different performance in terms of amount of energy stored, duration, efficiency, portability, etc. These include batteries, supercapacitors and flywheels amongst others. Current research focuses not only in fulfilling technical requirements but also in achieving affordable cost, sustainability and low environmental footprint.

Social and economic impact
Enhancing energy storage would enable flexibility to deliver energy *when* and *where* it is needed and to decouple generation from consumption. The main societal impact is related to the electric grid, as storage would allow maximizing the percent of renewable energies integrated. Some portable storage technologies, such as batteries, fulfil the technical requirements to power vehicles and have the potential to trigger electrification of transport, which would also greatly influence our current way of life. Both transformations would result in a drastic decrease in fossil fuel consumption and hence significantly reduce CO_2 emissions paving the way towards a greener energy landscape.

Involved teams
CSIC's research is aligned with European initiatives and its main strength is rooted in the Materials Science expertise. Current activities target both the improvement of existing technologies and the development of new concepts.

CHALLENGE 3

ENERGY EFFICIENCY AND HARVESTING

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1. INTRODUCTION AND GENERAL DESCRIPTION

Energy efficiency and Energy harvesting are two main topics in Energy nowadays. Mainly because in modern society, one of the key factors is energy-saving to become more independent of other resources. In this sense, two main approaches can be taken. On the one hand, behavior can be changed and thereby save energy. And, on the other hand, one can develop new technology able to save energy. In this sense, this chapter tries to give an overview of the situation of CSIC in Energy efficiency exploration.

Energy efficiency has always been a major challenge among scientists and engineers. However, in recent years, the increased public concern in the preservation of natural resources and the protection of the environment has strongly stimulated the research and development activities in this area. More than 200,000 technical papers written in 2019 and stored in “Scopus” database and more than 125.000 patents (according to google patents) having “energy efficiency” in their title, abstract, or keywords. There were around 30,000 publications and around 30,000 patents 10 years before. In the case of Energy Efficiency for buildings, the technology is on high TRLs, with many solutions already available and many companies involved.

A more recent concept is Energy harvesting. Less than 1000 papers use the “energy harvesting” in the title, abstract or keywords before 2009 according to “Scopus” and around 10.000 patents, while more than 33,000 articles have been published in really high-level journals in the last 10 years and around 10.000 patents according with "google patents". The reason behind this, is the interest of academia and industry in designing and engineering energy-autonomous electronic devices that can harvest energy from the environment and convert it to electricity to power devices. The development of energy-harvesting will be pushed in the coming years by the increasing need for autonomous wireless electronic systems and IoT in various fields of human activities, ranging from medicine, aeronautics, civil engineering, or animal tracking, to cite some. If wireless sensor networks could be powered by the energy available in the device's surroundings. This can make the Internet of thing (IoT) devices maintenance free and perpetually powered. Energy harvesting is still at the material and demonstration level in niche applications. But, at this level is where CSIC can still play an important role, with the critical mass of groups already in the field.

2. ENERGY EFFICIENCY IN BUILDINGS

Buildings are responsible for approximately 40% of EU energy consumption and 36% of the CO_2 emissions. Near 40% of energy lost in a building occurs through floors and roofs, 25% through windows and doors, and up to 35% heat loss through un-insulated walls. Buildings are therefore the single largest energy consumer in Europe.

At present, about 35% of the EU's buildings are over 50 years old and almost 75% of the building stock is energy inefficient. The construction sector is on its critical path to decarbonize the European economy by 2050, reducing its CO_2 emissions by at least 80 % and its energy consumption by as much as 50 %.

Investments in energy efficiency stimulate the economy, especially the construction industry, which generates about 9% of Europe's GDP and directly accounts for 18 million direct jobs. SMEs in particular, benefit from a boosted renovation market, as they contribute more than 70% of the value-added in the EU's building sector. In this sense, several paths are being followed nowadays to boost the energy performance of buildings. For instance, the EU has established a legislative framework that includes the amended Energy Performance of Buildings Directive (2018/844/EU). Together, the directives promote policies that will help:

- achieve a highly energy-efficient and decarbonized building stock by 2050.

- create a stable environment for investment decisions.
- enable consumers and businesses to make informed choices to save energy and money.

These challenges are addressed through the active innovation policies of the European Union. The Energy Efficient Buildings (EeB) Public-Private Partnership (PPP) is a joint initiative of the European Commission (EC) and the construction industry. This initiative aims at promoting research on new methods and technologies to accelerate the process of reduction of energy use in new and retrofitted buildings and to improve the European industrial competitiveness. The EC supported projects developed in the period 2010-17 demonstrate scientific and technological excellence, across the whole value chain, from early-stage conception to demonstration of almost ready-to-market innovations. The TRL of 168 research projects averages 6.4 with an average reduction of energy use due to the innovation of 31.6%. (EeB PPP Project review 2018).

2.1. Impact in basic science panorama and potential applications

A very important issue to define efficient strategies to increase energy saving in buildings is to take into consideration the society and environment in which we live, and adapt to it both the characteristics of construction-materials and novel construction techniques. In other words, it is important to take into consideration the actual society and climate in which we aim to apply these new strategies. For instance, there are some standards imported from northern Europe and even some regulations that propose to over-insulate the buildings to reduce energy consumption to zero. However, these standards should not be automatically applied to "benign" climates such as the Spanish one, where the interior of the buildings used to be in a temperature balance with the outside. The energy source per excellence in Spain, the sun, increases the temperature of buildings and partially accumulates in thermal mass, being lost in energy sinks (night, sky). In these benign climates, with well-oriented buildings (bioclimatic), there can be many days in which ambient heating or air conditioning is not required. So the technology must be according to the Spain climate. For example, if the building is over-insulated (as proposed in northern Europe), there is an important energy consumption increase for achieving a controlled atmosphere inside, and emissions to produce these materials and to recycle after their useful life are high. This does not mean that buildings should not be isolated, but it should be done properly and according to the particular circumstances of the area, to obtain effective isolation.

Or for example, in Spain, it cannot be used CO_2 gases for refrigeration as used in northern Europe because of the higher temperatures and there is still not a refrigeration gas adequate for our climate. Energy savings in a building can be also enhanced by using renewable energy sources, such as geothermal, for the building consumption, as well as the use of natural lighting with strict control over the quantity and quality of the light that gets into the buildings. This could be done through windows or transparent coverings, controlling the wavelength or the amount of light to reduce the energy consumption in terms of heating and cooling. Investments in energy efficiency may stimulate the economy, especially the construction industry.

Efficiently controlling the intensity and quality of the light that flows through the windows of a building is a very efficient strategy to reduce the energetic consumption without affecting the inhabitants' comfort. The basic principle consists of covering transparent closing surfaces with functional films able to control the amount and quality of transmitted light. This concept is typically referred to as "smart windows". Most solutions entail layers or multilayers with a maximum thickness of about one micron, in which each layer is responsible for a specific action (for instance, anode, cathode, and electrolyte in an electrochromic system). For this particular case, some of the most promising and currently investigated "smart windows" systems encompass the following:

- Low emission passive coatings: they let go through them the visible light but block the infrared, amounting to 40% of the total solar spectrum.
- Photochromic coatings: They automatically dark when irradiated with low wavelengths, usually in the UV-range. At present, they are not extensively used in buildings because their response depends on the UV irradiation and they are not easily applied to large areas.
- Electrochromic coatings: they change from transparent to colored, or opaque by application of a low voltage. They are currently used in last generation plane windows, and the technology is on the way of providing large area panels at a reasonable price.
- Thermochromic coatings: their transparency in the near-infrared changes with the temperature, and thus they can act as selective filters which automatically work when the surrounding temperature increases. This technology should be further developed for its up-scaling and its employ in buildings where transition temperatures should be adjusted to human comfort ranges, that is, between 21 and 31 º C.

- Gasochromic coatings: They change color when exposed to a certain gas, which is usually hydrogen diluted in argon. Nevertheless, the difficulties in making the process reversible and problems with the control of the gas makes that this technology is only at the proof of concept step.
- Improvement of natural lighting complements with developments in artificial lighting. The demonstration of electroluminescent semiconductors has enabled the widespread use of light-emitting diodes (LEDs) for illumination at lower energy consumption. However, the development of efficient LED lamps is bringing about an increase in lighting usage and hence light pollution, which may affect living creatures, from bacteria to mammals, that have evolved according to a day-night cycle. This concern:
- Need of reducing electricity consumption further by increasing control over brightness, color quality, and directionality of LED light emission, as well as to improve the performance of secondary optical elements guiding the light (mirrors, lenses, etc.).
- Commercial solid-state white light is generally achieved by the so-called phosphor-converted LEDs. The cold white light with a color-rendering index below 80 is inadequate for indoor lighting. Thus, novel white emitters are required.
- Complementary technologies like organic LEDs (OLEDs) and quantum dot LEDs (QDLEDs) offer several advantages such as the feasibility to develop thin, transparent, large-area, flexible devices. That will likely rise to new paradigms for its integration in buildings and to adapt their usage to passive natural lighting systems.

2.2. Key challenging points

New structural materials and new construction techniques

As it was previously mentioned, the construction process is responsible for an important part of the energy consumption associated with buildings and human structures. The new requirements, ever more demanding, and the scarcity of specialized labour, are driving the market to a more industrialized way of doing things. To meet the expectations, while reducing the energy needs, novel and more specialized materials and construction techniques are needed, such as:

- Advanced structural materials: concrete (Ultra-High-Performance Concrete, UHPC, more sustainable), ceramics, steel, glass, etc.
- Innovative materials for novel ways of construction: multifunctional

materials with advanced properties and performances: multifunctional concrete, photocatalytic materials, thermochromic materials, etc. These would lead to intelligent facades, better isolation, and solar control, for instance.

- Novel systems for construction: robotics, 3D printing, etc.
- Going back to nature, building with fewer resources and emissions, using natural materials, with low carbon print. Bioclimatic architecture.
- Efficient ventilation systems. Energy-efficient and energy storage systems (thermal and electric batteries). Thermal activation of the buildings, to take advantage of thermal inertia. Highly efficient cold and heat production systems from both the energetic and environmental point of view. High-performance heat pumps (aerothermal, geothermal, gas) sustained by solar thermal energy. More environmentally-friendly coolants. Novel systems for the capture and dissipation of thermal energy.
- Monitoring and control of the thermal and electrical conditions of the buildings. Maintenance of the well-being conditions.
- Connected buildings. Autonomous systems for energy production, centralized systems for heating. Intelligent and remote control for optimization of the conditioning systems.
- Building and city: conditioning of the urban spaces in a sustainable way.
- Efficient renovation of the existing buildings.
- Recycling and reusing of the construction materials. Evaluation of the sustainability of the products and buildings via the Cycle of Life analysis.

Novel functional materials to efficiently control passive lighting

Recent studies claim that reductions in energy consumption in commercial buildings using intelligent coatings (based on an electrochromic principle) could be around 30 to 40% in the next ten years. Increasing the penetration of these technologies will require concrete impulses both in fundamental science and in engineering innovations towards reliable and low-cost mass production. Increasing the lifetime of materials and their resistance to ambient conditions (air, light, temperature, rain, wind, etc.) will also be a central aspect of these technological innovations. The following R&D challenges are devised regarding the development of these novel processing methods and alternative concepts to control light:

- Thin-film methodologies can be easily scale up at low-cost large-area surfaces.

- Development of organic or molecular materials that combine durability and enhanced response to electric, thermal, or optical stimuli, fabricated by green chemistry processes.
- Novel formulations and architectures of inorganic or hybrid materials and a combination for their integration in smart systems providing faster and highly reversible responses over long cycling periods.
- Multifunctional coatings/systems based on a multilayer approach that presents effective responses to, for example, UV light, temperature, IR radiation, electrical stimuli.
- Integration with TIC technologies for an automatic and controllable response as an additional element within the "internet of things" concept.
- Development of mixed technologies that integrate light intelligent actuation and control with energy harvesting processes. An obvious choice is photovoltaic, but alternatives such as friction forces, raindrop, or thermal energy should not be disregarded.

Artificial lighting

Artificial lighting is an active topic of research in a double perspective, further increasing the energetic performance and light properties of the current LED technology and the development of alternative large-area devices for lighting. Although LED light sources are nowadays ubiquitous, they should address several key challenges in the quest for the next generation of emitting devices.

In terms of efficiency, the biggest challenge in inorganic LEDs based on GaN is the so-called "efficiency droop" or "efficiency roll-off", i.e., the dependence of efficiency on power input. Commercial white LEDs comprise several efficient blue LEDs made of different materials that suffer from this limitation. Thus, although state-of-the-art blue LEDs show electrical-to-optical conversion efficiencies around 50%, red and especially yellow and green LEDs feature efficiencies below 30% or 20%, respectively. Despite that some solutions have been proposed to improve efficiency for green light emission it is still a challenge to develop novel electroluminescent materials to overcome this so-called "green gap".

Beyond efficiency, developing light sources with expanded functionalities will open new avenues for the flourishing of LEDs. Applications range from visible light communication (VLC) to horticulture or healthcare. VLC uses light sources for both illumination and data transferring without cables, being the maximum bandwidth for communication limited by the rate at which LEDs can turn on/off. Emitters with fast radiative lifetimes should allow attaining white light sources with rapid response. However, since light has a great impact on human mood or productivity, the spectral composition of light and its flash duration should also be adapted depending on specific tasks or environments.

In addition to the proper LED sources, conventional optical elements relying on geometrical optics should be improved to provide better control over brightness, color quality, or directionality of LED emission. A possible option entails the combination of emitters with photonic nanostructures to maximize light output and to provide precise control of the radiation shaping in light-emitting devices.

Finally, **lighting devices based on solar radiation**, are indispensable, in countries like Spain. Apart from being environmentally friendly and reduce the consume of electricity. They present benefits to human life like well-being, productivity. And it is good on heritage conservation. Within natural lighting systems, tubular systems called light pipes or light tubes are developments to increase daylighting in interior spaces where natural light is minimal or absent. Light guides are considered one of the key renewable energy sources used in daylight transporting light long distances by reflections on their surfaces. The guide of light is designed according to many parameters like efficiency and health ambient. The possible drawbacks of this technology are that sometimes long distances are required and the absorption of the material using in the light pipes limits the guide. Or, for example, that due to space limitations the light guide must be bend resulting in a decrease of efficiency.

3. ENERGY HARVESTING

3.1. Impact in basic science panorama and potential applications

Energy Harvesters fall into two main categories: micropower generators, such as power sources for microelectronic systems (<W), and large-scale generators for large scale recovery of energy usually wasted in infrastructure, factories, or buildings (>W). In both cases, these systems are intended to harvest energy locally, by converting the environment sources available such as wasted head, friction, electromagnetic fields, etc.) into electrical energy that can be reused or stored.

The demand for microscale energy harvesters has expanded along with the Internet of Things (IoT) and wearables, expected to reach end-user spending about 1.567 billion $ (Statista, 2020), with a forecasted investment of 775 $ (in energy harvesters) in 2025 (MarketsandMarkets, 2020). This market is nowadays critically dependent on batteries, which hinders the full realization of the technology. On the one hand, the maintenance and recharging of batteries obstruct the remote and wireless application of a great part of these devices (for instance for the wireless sensor networks WSNs and health-care related self-powered sensors and actuators). And, on the other hand, batteries have a striking environmental costs. Aside from the ongoing change of paradigm in the automobile industry, pushing towards electrical cars. This will strongly affect the supply of raw materials for batteries, which are already scarce. Thus, there is a high interest of both academy and industry in the development of micro-energy harvesters and nanogenerators for IoT and wearables, mainly based on advanced materials and nanotechnology.

The recovery of energy at large scales is equally important as it has been estimated that at least 20% of the energy used in the industry is lost in vibrations and heat. The recovery of a few amount would have a transformational impact on the environment and economy. Thus, the role of scavengers from thermal and kinetic energies becomes prominent. Finally, the photovoltaic cells and RF harvesters should also be also mentioned as technology available to use for microscale power generation.

3.2. Key challenging points

Harvesting of mechanical energy –piezo and triboelectric-

Generally, mechanical energy (motion, vibration, stress, and strain) is available in e.g., buildings/constructions such as roads and bridges, operating machines, human bodies in daily activities, or sports, etc. and also at large scale. Some examples of mechanical or kinetic energy harvesters are for electrostatic energy harvesting (triboelectricity in triboelectric nanogenerators (TENGs), electrects), for piezoelectricity (piezoelectric nanogenerators (PENGs). And, also, electromagnetic transductors and electrostrictive and magnetostrictive energy harvesters.

Piezoelectric nanogenerators generally consist of the piezoelectric material sandwiched between the electrodes and interlayers to reduce losses that can undergo deformation or vibrations upon interaction with the local environment. One of the main advantages of this type of energy harvester is their high compatibility with micro- and nano-scale dimensions, making them especially appealing for the miniaturization of devices. Important challenges in PENGs deal with the optimization of materials from two points of view, the energy conversion performance and the improvement of the environmental compatibility of materials and device production.

Compared with piezoelectric energy harvesters, the utilization of the **triboelectric** effect to scavenge mechanical energy is a relatively new. The first reported is from 2012 (Wang, 2012). To date, *record levels of electricity generated with voltage/current outputs as high as kV/mA have been achieved* (Wu, 2019). A triboelectric nanogenerator TENGs includes two surfaces in contact-separation-mode. The extraction of current depends on the mechanical input, and surface nature and contact area, i.e. roughness. TENGs offer high flexibility regarding configurations and materials in comparison with other energy harvesters, which makes them very appealing and easily adaptable to harvest from the different forms of mechanical energy. There are several groups from CSIC initiating their research in this field and being a new and exciting research area with record levels of electricity generated it is a big opportunity for CSIC at this stage.

Challenges for Harvesting from motion, vibrations or mechanical –piezo and triboelectric-

As a whole, for the ample variety of kinetic energy harvesters, the near future research and developments around kinetic energy harvesters should focus on portability, scalability, and integration. Thus, the general challenges for this group of energy harvesters include:

- **Enhance the energy conversion capability for single-source kinetic harvesters and impulse the large power generation:** For piezoelectric approaches, the target in 2030 is to obtain over 1 - 1.5 mW/cm^3, for electrostatic, piezoelectric and MEMS (including low-frequency applications) and, 10 mW/cm^3 for electromagnetic transduction (NEREID, 2018). The fulfillment of this challenge requires further research on nanoscale advanced materials under design and the improvement of the implementation of these nanomaterials in devices without losing track of the requirements for a large scale and sustainable production. Besides, the performance for harvesting from random movements needs to be enhanced at several levels: random movement of humans for powering wearables, semi-random movement coming from structural materials in relationship with the loop forward towards large scale energy harvesting (with sources as steel frameworks, facades, roads and from waves in the oceans (blue energy)). At this point, it is also important to enlarge the overall frequency bandwidth of the electrostatic conversion at low-frequency targets (below 100 Hz), aimed at both large and micropower levels and applications. Moreover, the **development of flexible and low-cost devices,** including wearable devices, will take special importance when looking at the fabrication of affordable payback devices. The reliability and life cycling of these devices under real outdoor and wearable conditions need to be boosted, with the expectations to reach operation life over 10 years shortly**.** This issue is especially critical for electrostatic conversion and kinetic energy harvesters based in low dimensional nanomaterials. Besides, it is required research on the design of kinetic energy harvesters for harsh and hazardous environments, where the remote and wireless operation takes on special importance. The role of the development of simulation tools for optimizing kinetic energy harvesters will have a critical impact.

- **Develop low toxicity and non-rare materials based harvesters to avoid, for instance, lead-based piezoelectrics or rare-earth free magnets:** This will also positively affect the biocompatibility of the devices aimed at for medical monitoring and actuation and self-powered sensors. Alternatives such as ZnO, AlN, certain polymers, and lead-free ferroelectric ceramics are being intensively explored and will profit from the combination of the advanced protocols for materials synthesis and tools for materials design.
- **CMOS Integration:** As one of the most important applications of these energy harvesters is envisaged as a power source for smart devices, such as wearable devices, self-powered sensors, and actuators for large structures monitoring, security and health-care, their straightforward integration with CMOS technology is the nowadays and near future warhorse**.** Their integration is at the threefold level, as not only the combination of the energy harvester with the CMOS technology is needed, but also the energy storage system and the biological systems. In this context, it will be particularly demanding the development of ultra-low-power sensors and the corresponding non-conventional circuits for low energy power conversion and the optimization of sampling/sleeping schemes for low energy budget measurements.
- **Kinetic energy harvesters and circular economy:** In this context, the use of kinetic energy harvesters is not only limited to the reduction of

the dependency from fossil fuels and batteries but also addresses the use of kinetic energy harvesters as a tool for revalorization of plastics. In this case, cost-effective protocols for the modification of polymeric and plastic surfaces must be introduced within the production of piezoelectric and, mostly, triboelectric nanogenerators as an opportunity to generate added value from recycled materials.

- **Single-source hybrid integration and multisource-energy integration:** Hybrid energy harvesting technologies by combining sources, control, and storage elements. Single-source harvesters have not become fully competitive with batteries, and thus hybrid energy harvesters have emerged to simultaneously or individually scavenge different environmental energies using an integrated device. There are two strategies for multisource energy harvesting: Hybrid structural harvesters combine different single-source scavengers or to exploit different effects to harvest from a specific source. The main challenges for this approach concern the design of the devices (maximize energy conversion and minimize size) and avoiding interferences between the single-source harvesting effects. On the other hand, multisource harvesters rely on multifunctional single-materials or devices able to convert from different sources. This approach is yet in the emerging stage with room for exploring the best candidates from the advanced materials development perspective. Ideally, the material needs to be optimized to provide simultaneous efficient harvesting by different energy conversion effects and very few candidates fulfill this requirement.
- Develop **standard characterization procedures** and efficiency targeting: Addressing a target value for kinetic and multisource harvesters' efficiency would be appealing. However, contrary to the situation for solar cells, an international norm to evaluate the conversion efficiency in these harvesters has not been provided so far. The variety and random criteria for selecting working conditions, kinetic sources or multisource, fluctuations, etc. hinder a realistic comparison of output powers among the state-of-the-art results. We need to go beyond the figure of merits for cantilever piezoelectric conversion.
- Increase the **support to European industries** active in most of these concepts.

Harvesting from thermal sources

Thermal energy is everywhere, in natural and artificial environments. Examples of natural sources for thermal energy include the sun, the Earth's core, human body, etc. and of man-made (artificial) sources include transportation (combustion engines, exhausts), industry, etc. These thermal sources are normally not used. But, a temperature gradient can be convert into electricity using for example thermoelectric devices.

The current and next future challenges in thermoelectric approaches and devices are to maximize their efficiency and/or total power output, which are still modest. Thermoelectric endeavors have two complementary aspects: they have a material and thermal transport side and a device architecture and manufacturing side. Thermoelectric legs subjected to a temperature difference need to be built with such materials, and those legs need to be arranged electrically in series and thermally in parallel in devices, known as thermoelectric generators (TEGs). These two sides can be developed separately to a certain point, but eventually, efficiency, power performance, material availability, and capacity of integration need to be considered as a whole and sometimes traded-off. Therefore, one can divide the challenges in harvesting from thermal sources in two: material performance optimization and device improvement.

Challenges in improving thermoelectric materials

For a good thermoelectric performance (efficiency), thermoelectrics must have a unique combination of high electrical conductivity, low thermal conductivity, and a high Seebeck coefficient. Research should be focused on obtaining inexpensive materials with high conversion efficiency and stable in the temperature of application. The main paths for future research should be:

- **Design of high-performance TE materials** (Beretta, 2019) (Martin-Gonzalez, 2013)**:** Lowering the thermal conductivity by increasing phonon scattering. This is particularly relevant for inorganic semiconductors which exhibit good electronic properties, but sometimes high thermal conductivities. This can be achieved thanks to nanotechnology, either by decreasing the transport relevant dimension of the material by nanostructuration and creating a novel meta-material (with novel properties due to the nano-architecture) or by introducing scattering centers in the structure, without affecting its electrical transport. Some developments in this sense have been already achieved, such as nanowires of thermoelectric materials or even bundles of nanowires of not so good thermoelectric materials, such as silicon, which in the form of low dimensional structures achieve decent efficiency. In this sense, the research on designing and achieving low dimensional structures should be pursued, given that this could pave the way for achieving efficient meta-materials based on low-cost components.

- A deeper study of promising **novel materials based on non-toxic, sustainable** (abundant and available) and **less expensive elements**: There has been lately much research on materials such as silicon, silicon germanium, silicides, skutterudites, oxides, chalcogenides, etc., which can be further improved for thermoelectric applications by optimizing their charrier density or by decreasing the thermal conductivity.
- Deeper study on organic and inorganic semiconductors which can be used for **low to moderate temperature applications**.
- **Novel material combinations** for taking advantage of the wide thermal gradients available, in the case that there is not a single material with an optimum efficiency all along with the thermal range of interest. Therefore, segmented materials, where different materials, each optimized for a certain thermal gradient, are combined along the TEGs legs, are of interest.
- A novel, **cost-effective, and scalable** way of obtaining functional thermoelectric materials should be studied and further developed. Those include sputtering, electrochemistry, cold and hot sintering, 3D printing, screen printing, spray coating... which from a device integration perspective is interesting.
- Depending on the target application, novel solutions for ancillary materials playing a role in terms of thermal contacts, thermal isolation, biocompatibility, preservation of properties over a large number of thermal cycles, etc. are needed. For instance, if one thinks of achieving TEGs for powering wearable devices, the need for inexpensive and biocompatible materials for encapsulating the TEG, without degrading its properties, is clear.

In the case of organic thermoelectric, some specific challenges are ahead:

- Improve performance through the **increase in electrical conductivity**. For this, the first need is to understand how doping works in organic semiconductors, what are the doping mechanisms, what governs doping efficiency, and what changes are introduced by the dopants in terms of microstructure and thermal conductivity. There are also opportunities to decouple electrical conductivity increase leaving Seebeck unaffected by the structural control of charge carrier mobility (e.g. through polymer orientation).

- Improve performance through **decreasing thermal conductivity**. The solid with the lowest thermal conductivity is fullerene, which has just twice as much as air and almost one-tenth of a typical conjugated polymer. A general understanding of thermal transport in organic semiconductors would enable us to extend the case of fullerenes to other systems.
- **Improve stability**. Upon thermal stress, most molecular dopants sublimate, strongly decreasing the performance over time. Standardized testing of stability in organic thermoelectrics is yet to be developed.

Thermoelectric devices can be quite big, for heat recovery thermal management and efficiency-boosting industrial applications, or small, even miniaturized, for micro-scale energy autonomy provision in the **IoT scenarios**. In any case, the device architecture should maximize the percentage of the external existing temperature difference made internally available to the TEG legs for thermal to electrical conversion. There are crucial material and technological choices to be made from a thermal management perspective taking into account the different TEG elements (functional components as legs and ancillary ones as heat exchangers) and their interfaces. Similarly, the internal electrical resistance of the device should be minimized to deliver as much energy/power as possible by decreasing electrical internal losses. These aspects are common to both macro and micro-devices, but given their different final objective and that material behavior is mediated by scale factors, their architectural and design choices may differ.

- From a device building perspective, macro devices are generally *assembled* and micro-devices are generally *integrated.* Again, strategies may diverge, but for enabling TEGs being exploited beyond niche applications both approaches need to be sorted out through cost-effective and scalable technological procedures. For micro-devices, pairing thermoelectric technologies to mainstream silicon technologies is an enabling path to explore since the latter is already proven for scalability, miniaturization, massive parallelism, micromachining, and heterogeneous integration. This is boosting the interest in nanostructured thermoelectric materials as well as in a sustained effort for exploring the compatible processing of other promising nanostructures like 3D interconnected nanowires or other thin-films.
- Another interesting architecture are cascade devices, where different TEGs are assembled thermally in series and with independent electrical

circuits. These solutions are important when the harvesters are placed in environments with high thermal gradients, such as factories, or space applications.

- The electrical output of thermoelectric harvesters needs to be appropriately driven and controlled, especially in sensor powering scenarios in the presence of small thermal gradient such as sensors for healthcare, implantable devices, flexible devices smart clothing, building facades, IoT, etc. It is mandatory to develop the necessary electronics to convert the low energy obtained into usable electricity at a very low cost. Different applications for self-powered sensors will require different solutions that should be optimized in each case, taking into account that in most cases they may be connected to batteries.

Challenges in Thermal Management

One of the main challenges, to manage the harvested energy, is to combine them with rechargeable (secondary) batteries or capacitor-like storage devices, in such a way that a meaningful energy autonomous system is obtained. This will increase the window of operation in such applications. Hybrid approaches apart, new power sources with the ability to collect and store energy at low and zero cost, which would allow intelligent sensors to function autonomously maintenance, is both a challenge and a need.

Other key challenges of thermal control are related to the development of highly non-linear, switchable, and active thermal devices (Li, 2012). These devices are known as thermal diodes, switches, or regulators that are capable to manage heat in a way analogous as how the electronic devices control the electrical current. Despite their interest, these thermal components are still in its early stages and the contemporary thermal research is focused on exploring mechanisms that can provide these new capabilities.

Some novel thermal components for active heat control, like thermal valves, are based on mechanical or fluidic working principles. Nevertheless, the size of these devices is relatively large and their reliability is limited, due to the presence of moving parts. On the contrary, active thermal management devices based on solid-state are silent, reliable, and scalable. These features make them ideal components for thermal management in electronics or for the development of novel thermal technology based on heat logic. Nanotechnology has opened up new possibilities to develop materials with thermal asymmetry depending on the heat flux directionality (thermal diode) or high thermal variability in the material properties under some external stimuli, like electric or magnetic field (thermal switch).

In the field of thermal diodes, a certain amount of thermal rectification can be achieved by the union of two materials with strongly different thermal conductivities dependence on temperature. This is based on a classical Fourier law effect that was first observed in the 70s (Jerzowski, 1978). In the last few years, several nanostructures have been suggested to develop novel thermal diodes, like inducing nano-indentations that preferentially scatter phonons (Roberts, 2008), through different geometrical shapes (e.g. carbon nanocones) (Yang, 2008) or asymmetric mass-loading nanotubes (Chang, 2006). In the field of thermal switches and regulators, the most popular options are related to dynamic changes of matter, like phase change materials (Lee, 2017), that vary their thermal properties as a function of an external stimulus (e.g. electric or magnetic field, pressure, temperature,...). However, the thermal rectification and switching performances are still very limited impeding the progress of this technology. Future advances in the field of thermal management require novel materials, structures, and strategies that allow the development of active thermal devices with high efficiency. This is a relatively new research area where CSIC can play an important role.

4. INTEGRATION OF THESE TECHNOLOGIES TO POWER IOT, WEARABLES, AND SENSORS

4.1. Impact in basic science panorama and potential applications

The Internet of Things (IoT) is defined as a network of devices that are used to collect information from the environment and eventually, interact with it. The ability to monitor and manage objects in the physical world electronically makes it possible to bring data-driven decision making to new realms of human activity; optimize the performance of systems and processes, save time for people and businesses and improve quality of life. Potential applications range from environmental monitoring in different settings such as homes, offices, factories, worksites (mining, oil and gas, and construction), retail environments, cities, vehicles, and the outdoors to human body-centered systems that monitor health and wellness status or workers' productivity-enhancing applications (augmented-reality technology). The IoT is still in the early stages of growth. Every day more machines, shipping containers, infrastructure elements, vehicles, and people are being equipped with networked sensors to report their status, receive instructions, and even take action based on the information they receive. It is estimated that there are more than nine billion connected devices around the world, including smartphones and computers. Over the next decade, this number is expected to increase dramatically, with estimates ranging from 25 billion to 50 billion devices in 2025.

The nodes that configure the network consist of sensors, communication modules, and information processors. It is widely acknowledged that stable and reliable electrical power is needed to enable the correct functioning of the devices in the IoT scenario. If the power demands of ICT corresponding to data generation and storage are not decreased and optimized, it is expected that this sector will consume 20% of the entire world's electricity in less than a decade. In this sense, the implementation of renewable energy systems is mandatory to make IoT scenarios both sustainable and affordable.

Power sources for IoT devices can be split into two different categories (1) Energy scavenging and (2) Energy storage systems. Till very recently, state-of-the-art environmental sensing nodes such as temperature or fire detectors in houses or water/gas leak detectors in industrial sectors have been directly powered through AC lines, whereas mobile applications such as heart rate monitors or smartwatches make use of Li-ion rechargeable batteries that allow operational times up for several days. However, significant efforts have been made in the last years to develop miniaturize energy harvesting strategies that could eventually substitute wires and extend battery lifetimes. To make energy harvesting a suitable option to provide power to IoT devices, some challenges have to be assessed and overcome.

4.2. Key challenging points

- Generated net power: IoT has a wide range of power requirements depending on its functionality. Average consumptions are in the order of 1 to 10mW for sensing and processing functions whereas communication requires 100mW to 1W depending on the technology and the distance range of the signal. Generally, energy harvesting developers report power generation data normalized to area (solar harvesting), or volume (mechanical, thermal). However, Although IoT nodes for stationary applications can integrate relatively large power sources (~ 100 cm^3), portable and wearable devices should be light and small (~1-10 cm^3) and adjust to the device form factor. This prevents some energy solutions from being implemented in real applications of the IoT arena.

- Generated voltage requirements of electronics modules of IoT devices set a minimum of 1.5V (if not higher) to operate. The output voltage of some harvesting sources is generally insufficient. Exploration of device architecture that makes possible cell stacking is urgently needed. Required targets of minimum operative voltage are set by the minimum voltage required by commercial DC-DC voltage converters (100 mV).
- Reliability and manufacturability is at their earlier stages of new material solutions as a criterion to discriminate and assess the real applicability of their materials in the IoT arena.
- Energy harvesting systems, except thermoelectric, fail in continuously generating power as the environmental energy source (sun, mechanical movements...) may vary along the IoT operating time. Therefore, some form of energy storage is required if power demand is to be fulfilled at all times. Energy storage is currently being dominated by batteries and capacitors. Synergies of research groups between energy harvesting and energy storage would be very beneficial to render material and device development operative.

5. CONCLUSIONS

CSIC is not without constraints itself, and the way it should engrain in the Spanish Public R+D system is not a closed issue in these post-agency days, but it should do its best to help promote research avenues were instrumental, if not excellent, contributions can be made. Breaking the walls of the former Knowledge Areas to ease cross-fertilization and synergetic endeavors is the first point, breaking virtually the institute's walls would be a second one: a more interwoven CSIC fabric is needed for tackling the challenges of the future. And that can be articulated by internal CSIC projects where the different CSIC groups can collaborate in the same framework.

Funds at the reach of CSIC researchers are regional, national or European. With different intrinsic features, all share some limitations that prevent fruitful concurrent participation of different CSIC institutes. Regional instruments tend to be quite transversal, but with too thin budgets per participant and with adverse participation (justification) schemes for CSIC institutes. National projects offer limited resources making a multi-institute CSIC participation risky. European based projects offer a wider CSIC institutes participation, within a different order of magnitude of limited resources, but where the country share should not overshoot, and the cost-benefit of application to oversubscribed calls is increasing painfully. In the end, restricted cross-participation limits overall research transversally and overall transcendence.

It would be wonderful if CSIC itself could fund in stable way networks of groups of different institutes collaborating in mid-term and long-term projects. However, if managing its research funding is beyond the grasp of CSIC, the institution should try to provide the appropriate connective tissue among the institutes that may share a given challenge to help them align and integrate their strategies.

Today, scientific research management is favoring mission-oriented, thematic platforms arrangements that embrace 'big problem' solving goals by the vertical connection of actors and backgrounds. Enabling-horizontal-endeavours (such as energy harvesting) may not find easy accommodation in this new scheme since they do not fit one but many of those vertical approaches. In these cases, maybe generating virtual institutes to get together groups working on similar subject can also be a possibility to be consider to group similar interest. It must be stressed that enabling-horizontal-endeavors needs similar encouragement and nourishment, and a support scheme of their own, to be profitable.

In any case, energy efficiency, energy harvesting, and IoT powering are subject in which CSIC can performed important contributions. Mostly in the subject that are starting and do not have very high TRL yet. But an effort in networking those groups and stablish project for the groups to collaborate will make the contributions to the fields much stronger than having separate groups working by their own.

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TABLE 1—List of challenges to be addressed for the Challenge 3

		NEAR TERM (<5YEARS)	MID TERM (5-10 YEARS)	LONG TERM (10-20 YEARS)
ENERGY EFFICIENCY IN BUILDINGS	**New structural materials and construction techniques**	• Novel advanced structural materials for construction: thin films, multifunctional coatings, integration with TICs, etc. And methodologies: 3D, printing, etc.	• Scalable and advanced processing methods to take to higher TRLs and exploit these materials for smart windows, energy-saving facades, new approaches for energy storage.	• Multidisciplinary approach to novel functional materials to control ligth through windows, construction coatings, etc.
	Artificial lighting	• Improvement of LEDs (reduce power consumption andenvironmental impact, increase brightness), commercial solid state white ligth emmitters, related technologies like OLEDs or QLEDs	• Higher integration with industrial activities: advanced and scalable processing methods for artificial lighting production.	• Novel materials and effective devices to improve the use and integration of the generated artificial light in buildings
	Functional materials for passive lighting	• Development of new material formulations compatible with simpler manufacturing techniques and applicable to large areas	• Up-scaling the technology for large ara applicactions. Integration with current manufacturing procedures. Increase of automatization control and connection with TICs processes.	• Multifunctionalitiy and integration with photovoltaics and other energy recovering systems.
	Efficient Buldings	• Efficient ventilation systems, thermal activation of buildings, passive lighting	• Connected buildings, conditioning urban spaces in a sustainable way, contruction and demolition waste management	• Automatic control systems (sensors and actuators) connected to the information network.
ENERGY HARVESTING	**Mechanical energy harvesting**	• Improving portability, life-time, scalability and integration of kinetic energy harvesters (piezo and triboelectrics).	• Enhance energy conversion, development of flexible and low cost devices based in low toxicity and non-rare materials. Development of standard characterization procedures.	• CMOS integration, circular economy, single source hybrid integration and multi-source energy integration.

		NEAR TERM (<5YEARS)	MID TERM (5-10 YEARS)	LONG TERM (10-20 YEARS)
	Harvesting from thermal sources	• Maximize efficiency and/or total output through high performance TE materials, better thermal contacts/ isolation, and endurance in assembled macrodevices, integrated microdevices.	• Novel TE materials combinations based on non-toxic and abundant elements. New developments (size, flexibility, biocompatibility) to explore further embedded/ditributed applications: clothing, building facades, IoT, etc.	• Further research on thermal management (novel materials, structures and strategies) and on the economics and manufacturing scalability of all sort of device footprints and temperature ranges
IoT POWERING, WEARABLES AND SENSORS	**Energy scavenging and storage**	• Miniaturization, increasing of the voltage output to reach 1.5 V (in most cases), reliability and manufacturability	• Multidisciplinar approach, novel materials and architectures and more interactions with industry.	• Research to industry transference (and to society)

CHALLENGE 4

INDUSTRY ELECTRIFICATION AND GRID MANAGEMENT

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1. INTRODUCTION AND GENERAL DESCRIPTION

In recent years, big efforts have been devoted to reach a complete electrification of buildings (heating and air conditioning, lighting, etc.) and transportation (electric vehicles, railways, more/all electric aircrafts, ship propulsion, etc.), but **industry** is one of the most difficult areas to electrify. Electrification, in this framework, means replacing technologies and processes that do not use electricity with ones that do, for example, substituting natural gas furnaces for electric-powered heat pumps. With the rapidly falling cost of solar photovoltaics, wind power, and battery storage, **industry electrification** coupled with renewable electricity supply has the potential to be a key pathway to achieve a deep decarbonization of our society, as the industrial sector accounts for up to 30% total CO_2 emissions and 25-30% of the global final energy use (Banerjee 2012) (European Commission 2018). In Europe, around 30% of that energy is electrical and only about 7% comes from renewable sources (IRENA 2018). Consequently, there is still a huge margin for increasing the use of zero-emissions electric energy in the industry. It has been estimated that for achieving the CO_2 emissions target for 2050, the electric energy from renewable sources used in industry must increase from the present 7% up to at least 48%, and the total energy used from renewables (including biomass) must reach 68% (IRENA 2018). This approach is in line with the European Green Deal, including Key Actions on "Clean, affordable and secure energy" and "Industrial strategy for a clean and circular economy" ("Initiatives to stimulate lead markets for climate neutral and circular products in energy intensive industrial sectors"). (European Commission 2019). Industry is the most challenging sector to decarbonize due to the energy demands (mainly in form of fuels for heating) of certain energy-intensive industries, the high carbon content of certain products, and the high emissions of certain processes, making innovative solutions necessary. In addition, the industrial transition to electricity will be only undertaken by companies if it is economically beneficial (Guminski 2017), playing out differently in different sectors, and depending on the development of different technologies (Brolin 2018). For this reason, accurate feasibility studies are required for each sector. For example, chemical, petrochemical and steel are among the largest emitters, because they employ energy intensive and high temperature processes difficult to decarbonize (IRENA 2018).

Considering 2015 data, around 77 % of industrial CO_2 emissions in Europe came from heating processes obtained by burning any kind of fossil fuel (45% from furnaces, 21% for obtaining steam and hot water and 11% for heating spaces) (Herbst 2018). Consequently, electrification is very promising for **industrial heating** applications (Schüwer 2018) (Guminsky 2019), as it enables both, high and low process temperatures to be achieved in a tailored and efficient way and enables the utilization of other energy sources like waste heat, geothermal or ambient heat (via heat pumps). Concerning electro-heating, one can consider two scenarios. In low temperature applications, heat pumps (up to 150ºC) and electric boilers (up to 300ºC) show a big potential (it is estimated that 6% of total heat in the industry can be provided from heat-pumps in 2040). On the other hand, electromagnetic heating technologies are suitable for a number of industrial sectors, sometimes involving high temperatures (Vairamojan 2018). The interest for electromagnetic heating lies in the fact that heat is mainly induced or generated in the processed materials via an electromagnetic field, avoiding any heat transfer mechanism (convection or conduction) between the heating element (furnace, oven, hot-plate,...) and the processed material. Although in some studies the impact of the electromagnetic heating technology is underestimated, other works consider that electromagnetic approaches could potentially reach 50% of the final energy demand for the European process heat (DECARB 2017). Some electromagnetic heating technologies (induction, infrared, resistive, electric-arc, radio-frequency, microwave) are relatively well established although they show high potential for application in different fields and there is still a large margin for improvement (for example in terms of efficiency) using new technologies such as superconducting induction coils and power electronics driven supply circuits. Other electromagnetic heating technologies (laser, electron-beam, plasma-arc heating) are emerging in the industry and require further research and development (De Keulenaer 2018).

Among the total amount of CO_2 emissions in Europe, 23% come directly from industrial processes (mainly chemical and non-metallic minerals sectors: production of ammonia, lime, bricks, cement clinker,...) and not from any heating action (Herbst 2018). Thus, direct **electrification of processes** has also a high potential, although there are not transversal technologies to be widely applied and each sector needs a particular solution. Today, electrified industrial processes are deployed in the non-ferrous metals and chemicals industries, while some further potential exists in the chemical sector (electrochemical processes) and in the iron and steel sector (steel electrolysis). In case that processes can be electrified, the emissions reduction potential is very high, assuming carbon free electricity. Ideally, the electricity surplus from renewable sources can be electrochemically stored in the chemical bonds of different species with added value that could, additionally, be converted into industrially important products, such specialties, commodities or fuels. Hence, the development of **material processing** and **electrochemistry technologies** will result in the creation of economic, environmental, and social value for many industrial sectors in a sustainable manner. Further research is required to increase the technology readiness level of these solutions.

Some of the most relevant industrial processes to be electrified in the 2050 horizon are:

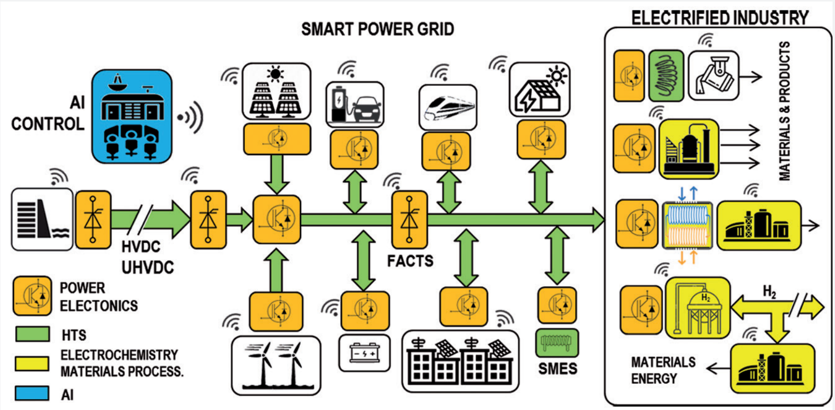
- Using electrolysis to produce hydrogen for replacing coke in the iron and steel industry and as a feedstock in the petrochemical industry (and also as energy carrier) (Brolin 2018)
- Electrochemical catalytic reactors in process industry (chemistry and pharmaceutical) (Schiffer 2017) (Serra 2019)
- Electric/hybrid boilers in the pulp and paper industry (Brolin 2018)
- Electro-thermal technologies for heating and drying (Brolin 2018)
- Electric arc heating (steel industry) (De Keulenaer 2018)
- Induction heating (including superconducting coils) (De Keulenaer 2018)
- Dielectric heating using RF and microwave generators (ceramics processing, paper and cardboard, etc.) (De Keulenaer 2018) (Schüwer 2018)

- Direct resistance heating (metal matrix composites) (De Keulenaer 2018)
- Electron beam heating (De Keulenaer 2018)
- Ultraviolet curing/heating of wood products, paper and printing (Jadun 2017)
- Steelmaking through direct electrolysis of the iron ore (electrowinning). (Philibert 2018) (Lechtenbohmer 2016).
- Electromagnetic forming by using high field magnetic pulses (Satonkar 2019).

As it has been shown, there is a clear potential for research and development in a variety of technologies allowing deep industry electrification. As it has also been mentioned, this target depends on the parallel implantation of renewable energies (some of them already discussed in this work). Nevertheless, another key point to be solved is the level of electricity demand and its availability (transport, distribution and conversion) required to reach the industrial decarbonization objectives for 2050: could the power sector provide such quantities of electricity in an economic and reliable way? Several models and roadmaps estimated that the total industrial electricity demand in 2050 required for production of feedstocks, clean gas (such as electrically synthetized methane) and hydrogen ranges between 2100 TWh and 4000 TWh (European Commission 2018). One of the added difficulties to estimate the projected consumptions for 2050 is that, although electricity will be the dominant energy carrier, electrification is not the unique option to reach a decarbonized industry. Other actions oriented towards CO_2 emission reduction are: the improvement of energy efficiency in present processes, switch to CO_2-neutral fuels (biomass and alternative renewable fuels), innovative low carbon processes, carbon capture sequestration and/or use, resources efficiency/circular economy, industrial symbiosis and material substitution. The level of implantation of these initiatives will modulate the electrification requirements in the different industrial sectors and in any case, the highest decarbonization expectative for 2050 will be only achieved if all mitigation options are exploited simultaneously.

The increased electric energy demand in the “more electric industry” is likely to go hand-in-hand with increasingly **flexible use of electricity**. In some cases, such as the production of hydrogen or process media, this flexibility will be in-built since the storable energy carriers create new production planning options. In other cases, new approaches to planning, process design, and the

FIGURE 1—Scheme of the smart power grid, allowing optimum, efficient, flexible and robust interconnection among all the elements of the future electric system based on CO2-neutral energy production and deep electrification (including the industry). The main fields involving CSIC group's research activity are represented.



use of automation may allow matching electricity use to favorable market and production conditions. The expected high penetration of intermittent renewable electricity in the power system may create incentives for this flexibility. In this scenario, the development of **smart power grids** allowing a two-way information and energy flow will be mandatory to support stability in both transmission and distribution networks (Brolin 2018) (ETIP 2018). Smart grid management based on power electronics conversion, efficient energy transmission and storage, communications and digital technologies will help to improve demand forecasting, enable self-healing from power disturbance events, facilitate active participation by consumers in demand-response mechanisms, and provide resilience against physical and cyber-attacks, improve quality of power, allow easy integration of renewable sources into the grid, foster innovation to enable new products, services, and markets, assist in optimization of assets, and improve operating efficiency (Bush 2013). In conclusion, the future electric energy system will rely on much higher balancing capacities, including flexible generation units, increased demand response and conversion, transmission and storage technologies, together with better interconnections at all grid levels (ETIP-SNET 2020). Concerning electric power conversion and transmission, as well as chemical processes electrification, CSIC has several research groups working on the key enabling scientific and technological disciplines supporting their development: power electronics and high temperature superconductors (both included as research areas in the ETIP-SNET R&I Roadmap 2020-2030 and in the Spanish Electric Grid Technology Platform 2030 vision document), as well as materials processing and electrochemistry (identified by the A.SPIRE Team in their 2050 vision document).

1.1. Power Electronics

Across the whole power supply chain between the (renewable) energy generation and its final use (industrial processes), a number of electric power conversion stages are required (FutuRed 2016). The electric energy from high-power plants (hydraulic, nuclear, etc.) is transmitted at high AC voltages (HV, > 30kV, 50-60 Hz) for long distances (< 1000 km). Power electronics circuits based on semiconductor power devices (mainly Silicon thyristors, diodes and more recently IGBT transistors) are used in order to stabilize and compensate unbalances in the transmission lines: the FACTS (flexible alternating current transmission system). On the other hand, HV DC lines have been also introduced in the past years for long distance (> 1000 km) bulk-energy transmission due to their significant benefits in front of traditional AC lines (lower losses, mainly in submarine and underground lines, asynchronous coupling, etc.). These lines allow intercontinental connections which could help to deal with the fluctuations of wind power and photovoltaics. At both sides of the HVDC line, power conversion stations based on semiconductor power devices are also used (Alassi 2019). In the final distribution segment of the smart grid, where renewable resources inject the energy and industrial loads use it, medium voltages (up to 30 kV) are involved. High power, bidirectional power flow converters known as Solid State Transformers (SST) are used in order to assure the voltage, current and frequency conversion determined from the higher level control of the smart grid (Kolar 2014). Finally, at the industrial power plant, different power converters are required for each specific process. Let's mention for example AC/DC converters supplying with 6.5 V and 50 kA electrolytic Copper foil fabrication lines (Luo 2015), the AC/AC MW range converters used in the steel industry (rolling mills, induction heating and melting, etc.) (Chattopadhyay 2010) and the high switching frequency DC/AC resonant converters (developed by the Spanish company GH Electrotermia) used in induction heating processes in the ceramic tiles industry (DECARB 2017). The basis for all the power conversion systems described above and their main enabling elements are efficient and reliable semiconductor power devices based on nano- micro-electronics technologies (Millan 2014). Semiconductor power devices are present in virtually all electric energy conversion process, and their development will not only boost industrial electrification: many other sectors (buildings, transportation, etc.) will also benefit from new generations of power devices, mainly based on wide band-gap (WBG) and ultra WBG (UWBG) semiconductors (Matallana 2019).

1.2. High Temperature Superconductors

High temperature superconductors (HTS) are key materials to reach the high efficiency and security required in electrical grids. They will provide unprecedented improvements in the **energy transmission** and distribution lines and some **industrial actuators** such as AC inductive heaters (Del Rosario 2013) (Casals 2009). High-capacity grid HTS transmission cables (from 35 kV-77 MVA to 66 kV-200 MVA) and the corresponding Superconducting Fault Current Limiters (SFCL, up to 450 MVA) will ensure energy savings and facilitate the integration of renewable energies in a flexible smart grid electrical network. Industrial electrification will be also enhanced through the use of energy storage systems like the Superconducting Magnetic Energy Storage Systems (SMES) (from 100 kW to 10 MW) in industrial parks. In addition, apart from allowing power transmission, HTS technology will also enhance industrial electrification thanks to direct drive motors or actuators with lossless and no friction parts, lighter wind generators (5-10 MW), more efficient mobile transportation (aviation, ships, trains) cables (12 MVA- 6kV), generators (10 MW)) and motors (from 100 kW to 2 MW). All these initiatives need to be coupled with the use of low cost cryogenic liquids or cryogenerators. In order to enhance the cooling power at lower cost, hybrid cryogenics has been suggested and developed. The abundance at the industrial level of cryogenic liquefied gases, as liquid Natural Gas, liquid Oxygen and liquid Nitrogen, has been considered as medium temperature ranges for cooling or screening cables, SFCL and some rotating machines. This medium temperature allows substantial decrease of the heat load. Cryogenerators, also called cryocoolers, based on thermal expansion cycles with cooling powers in the range of tens to several hundred of Watt are able to achieve low temperatures (20-40 K) for their use in motors, generators and SMES. Also the possibility to use them for medium temperatures as heat rejection level, leads to a substantial enhancement of the efficiency of that cooling machines (EASE-EERA 2016).

1.3. Materials processing and electrochemistry

Energy supply in the chemical industry is mostly based on fossil resources. With an increasing share and a possible cost reduction of renewable electricity, driving reactions using electrochemical conversion can be an opportunity for the chemical industry to reduce its carbon footprint and, in future, rely exclusively on renewable resources. This "process electrification" can be applied in different industries such as steel, non-ferrous metals, cement and lime production and in chemical and petrochemical industry. In addition, these reactions can consume CO_2 or produce H_2. Often, electrochemical reactors have no GHG emissions at all (when renewable electricity is used), and they do not produce waste that would need landfilling. Besides, separation operations, which are essential in chemical and petrochemical processes, currently rely on separation technologies that are energy-intensive and can represent up to 50% of energy consumption in chemical plants. In this sense, electrochemical membrane reactors (ECMR) allow the selective transport of ion species across the membrane controlling the composition in a reaction system. This highly efficient technology also offers the possibility of using less intensive and harsh conditions for the products formation regarding traditional thermochemical processes. The electrochemical separation offers the potential to replace the high thermal energy demand of distillation by much lower electricity consumption, at the same time eliminating GHG emissions. A wide range of electrically-driven separation technologies are being developed for a wide range of applications such as H_2 production by electrolysis and electrochemical membrane reactors (Duan 2020). One of the key advantages of electrochemistry is the process intensification. The ability of performing cascade reactions with simultaneous removal of the desired species from the reaction media, together with the fact that sustainable energy sources can be coupled to the process, and the possibility of using unconventional forms of energy, e.g. microwaves (Serra 2020), ultrasound, plasma, make this efficient and flexible technology a promising candidate to become one of the robust foundations on the industry electrification field.

2. IMPACT IN BASIC SCIENCE PANORAMA AND POTENTIAL APPLICATIONS

The industrial electrification challenge aims at transferring as much as possible industrial processes based nowadays on burning fossil fuels, to zero-emissions electric power based processes. The research involved in achieving this objective is, by definition, applied, very interdisciplinary and based on heterogeneous technological fields (semiconductor electronics, high temperature superconductors, electrochemistry, smart grids management). Nevertheless, for achieving the technological breakthroughs required for deep industrial electrification, scientific progresses must be achieved:

1. Power electronics is one of the main key enabling technologies required for achieving a deep electrification of the industry. The most challenging element to be developed in this field will be high power modules implementing the switches required in the conversion circuits, probably based on WBG and UWBG semiconductor power devices (see the section "Key challenging points"). With SiC technology well established for "low voltage" devices (below 10 kV), the first research works on Diamond have started few years ago aiming at developing very high voltage, current and operation temperature transistors (breakdown voltages above 15 kV, working temperatures above 300ºC). Other UWBG semiconductors such as Ga_2O_3 recently appeared as candidates for the development of the required power switches in flexible and high-power capability smart grids, although they are in the first stages of material research. In addition, other key factors affecting the development of this new generation of high power devices must also be considered. First, the packaging and characterization of these devices has become another challenge boosting the research on new materials and assembling methods. Second, there is a lack of characterization tools specifically devoted to the analysis of the electro-thermal and reliability issues of this new generation of devices. In conclusion, the development of new **high-power devices** based on **WBG** and **UWBG semiconductors** will rely on **significant scientific and technological breakthroughs explaining their physical behavior, specific nano- micro-fabrication technologies, advanced characterization methods and new packaging processes and materials**. These scientific achievements will have an impact not only on the applications foreseen in the industrial electrification context, but also for all the possible applications of power semiconductor technologies (automotive, space, aeronautics, naval, communication and data processing base stations, consumers, etc.).
2. More efficient power HVDC transmission/distribution lines, and protection fault current limiters will be obtained by the development of new HTS materials, which will be crucial for the electrification of industry. The design of such materials based on cuprates nanocomposites ($REBa_2Cu_3O_{7-x}$, RE=rare earth, with segregated oxide

nanoparticles) with specific characteristics will rely on the **research results about the physical and chemical properties of these quantum materials**. Nanoscale structured superconductors are a novel class of materials enabling an extreme technological push boosting a new generation of superconducting systems and devices with unprecedented performances. Reaching the ultimate performance through nanoscale control of composition, structure, shape, dimension and conductor architecture is still an outstanding scientific challenge. New progress in understanding the vortex matter physics is also necessary to approach the fundamental limits in critical current performance, which includes determination of the optimal carrier density by oxygen overdoping. All these efforts need to be implemented in long length coated conductor manufacturing scaling processes (in the range of km). Thus, the decrease of the cost/performance (€/kAm) figure of merit of the conductors is a key objective to achieve a high market penetration. This requires additional efforts in developing cost-effective processing methodologies which should then be scaled to an industrial production beyond thousands of km per year.

In order to integrate HTS materials into devices it has been mandatory to evaluate additional properties, like the mechanical strength, AC-losses, quench protections, electrical insulation materials and cryogenic compatibility. Further effort needs to constantly be done in these directions specially addressed to the device level for each particular application. So, not only experimental characterization but also multiscale simulations are being undertaken. In particular, for cables and SFCLs, it is mandatory to analyze the heat transfer capacity, maximum over-currents for a particular current rating, maximum sustainable electric field, etc. These scientific and technological achievements will have an impact not only in the application of HTS for electrical grids, but also for all the possible applications of superconductors and also for improving the knowledge of basic physical mechanisms in material science.

From the point of view of HTS applications, the conditions in which the superconducting material should work (temperature, magnetic flux density, current density and mechanical strain) define the working frame. So, **computational tools** are a key topic of research to get an optimized design taking into account the non-linear behavior of HTS materials. On the other hand, **low AC-losses** are needed in certain applications. Motors are limited to lower speeds, and SMES to lower discharge rates if AC-losses increase, thus thinner and narrower wires in the range of a tenth of millimeter are required for high magnetic rate cycling in high performance AC fast devices. Thin wires allow also a better strand transposition for high-current flexible conductors for high-current applications. Finally, **superconducting joints** is an additional challenge to be tackled since manufacturing lengths are limited to few hundreds of meters (500-600 m) with acceptable homogeneity. Nowadays, metallic joints with resistances in the range of 20 to 50 $n\Omega*cm^2$ are used. Finally, the search of **dielectric materials** with high electrical strength and high thermal diffusivity is also a topic of research to improve **electrical isolation** in large multi-turn coils for generators and SMES.

3. The integration of electrochemical processes in industry is attractive due to their energy efficiency, high yield and modularity. In addition, electrochemical processes can easily use clean and renewable electricity sources. One of the most attractive options available to electrify the chemical industry and promote sector coupling is the use of **electrochemical membrane reactors**. An electrochemical membrane reactor combines the properties of the electrochemical reactors, that use electric power to supply the energy for a chemical reaction, and the membrane reactors, that consist in multifunctional units combining a chemical reaction with a membrane-based separation. Then, an electrochemical membrane reactor transports substances controlled by galvanic operation and allow the chemical equilibrium displacement with the subsequent increase of the conversion yields and the reduction of the by-product formation. In addition, the integration of the sequential steps in a single unit allows thermal coupling, giving rise to an increase of the energy efficiency and decrease of the operational and capital costs. One of the main advantages of this technology is the possibility of **convert low energy molecules,** such as CO_2 and H_2O, **into fuels and chemicals** by using the surplus of renewable energy.

   Several advances have been made on the field in the last years, but there is still room to improve materials, components and devices. Further utilisation of electrochemical processes would require the **development of new catalysts, electrodes and compact electrolysis cells**. The progress in electrodes, electrolytes, catalysts and key enabling components (such as current collectors, manifolds, cell holders and seals) will be linked to the development of **novel materials and composites**, as well as **novel advanced manufacturing techniques** that allow controlling their **nanostructure and interfaces**. The resulting breakthroughs will have an impact not only in electrochemical applications but also in other materials science fields.

Other research areas involved in the industrial electrification process, will achieve significant scientific results covered in other sections or chapters of this work (e.g., artificial intelligence, digitalization, energy storage, renewable energy sources, etc.).

3. KEY CHALLENGING POINTS

1. Electric power conversion will be required among the different elements of the smart grid supporting the "more-electric industry", in order to adapt the voltage, current and frequency levels required in each element of the chain (e.g., solid state transformers). Power electronics converters will be also necessary to ensure functionality, control and stability of transmission lines (FACTS) and final processes (induction heating, electrolytic processes, AC drives, etc.). All power converters are nowadays based on Silicon semiconductor power devices. This material has reached its ultimate limits in terms of maximum voltage, current, switching frequency and temperature capabilities and the next generation of power semiconductor devices will rely in WBG and UWBG technologies (Veliadis 2018) (Wilson 2018). Recently, the first "low-voltage" WBG devices became commercially available (up to 1.7 kV SiC and 650 V GaN transistors and rectifiers, with working temperatures below 200ºC) and the first research works on Diamond have started few years ago aiming at developing high voltage, current and operation temperature transistors (breakdown voltages above 15 kV, working temperatures above 300ºC). The requirements for higher voltages are driven by the need of lower transmission currents, mainly in HVDC and Ultra-HVDC lines, while higher operating temperatures provide more robust devices and lower thermal management (cooling) requirements. Nevertheless, the target for commercially available power modules avoiding the limitations of the present Silicon-based high power devices (mainly rectifiers and thyristors) is still very far. Apart from SiC, GaN

and Diamond, new materials appeared in the UWBG semiconductors arena (such as Ga_2O_3) as candidates for the development of the required power switches in future flexible and high-power capability smart grids. The practical use of this new generation of high-power devices will require their assembly in power modules ensuring a correct electrical, thermal and mechanical interface between the brittle semiconductor layer and the external high power circuitry. In this sense, research on new packaging materials and assembling methods managing very high electric fields, temperatures, thermal conductivities and tailored coefficients of thermal expansion is required (Johnson 2018). In addition, the development of new devices is systematically associated to unknown physical phenomena and failure mechanisms that require very specific characterization tools, sometimes based on new measurement principles (for example, based on optical effects) (Perpiñà 2017). The experimental assessment of the new devices using appropriate tools is not only required for obtaining their operational electro-thermal response, but also for characterizing their reliability behavior. In conclusion, the key challenging point for the power conversion systems required in massive industrial electrification, is **the development of new high-power modules based on WBG and UWBG semiconductors, with their specific packaging and characterization techniques**.

2. In the field of efficient transmission lines based on superconductor materials, the main challenge is **to understand the physical and chemical properties of HTS quantum materials** in order to allow the design of new materials and conductors with specific properties to improve the transmission lines efficiency and smartness and to boost the electrification of industries (Obradors 2014). A key advantage of HTS power transmission systems is that they can carry higher currents without losses and so cables can achieve similar power rates without the need of achieving very high voltages (replace 220 kV lines by 35 kV ones, for instance), thus simplifying the whole electrical transmission grid. The high-level engineering reached at the nanoscale in HTS materials and recent breakthroughs in the physics and preparation methods of these materials, as well as the simulation tools developed to predict the behavior of these materials in real devices, are excellent instruments for addressing this challenge. Nanoscale structured superconductors are a novel class of materials enabling an extreme technological push boosting a new generation of superconducting systems and devices with unprecedented performances. Reaching the ultimate performance

through **nanoscale control of composition, structure, shape, dimension** and **conductor architecture** is still an outstanding scientific challenge. New progress in **understanding the vortex matter physics** is also necessary to approach the fundamental limits in critical current performance. Finally, the **understanding of the electromagnetic-thermal-mechanical behavior** is crucial for the integration of HTS materials in real devices.

3. Despite electrochemical membrane reactors are gaining interest in the last years, their industrial application remains still far away due to different challenges. This emerging technology needs deep **investigation in materials** that fulfil all the requirements to be introduced in industrial applications. Electrochemical membrane reactors are composed by a **membrane** and two **electrodes**. The membrane (also called electrolyte) must possess negligible electronic conductivity under the operating conditions as well as chemical and mechanical stability. Electrodes must be compatible with the membrane and they should present high electrochemical and catalytic activities. Finding materials that meet these requirements is not trivial and an exhaustive fundamental and experimental work is still needed. On the other hand, development of **efficient current collectors** with low cost is essential for commercial applications.

   Another key challenging point for the commercialization of electrochemical membrane reactors is the upscaling of the different components. Finally, lowering the process temperature down maintaining efficient transport properties and catalytic performances is also an important challenge to be overcome.

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TABLE 1—List of challenges to be addressed for the Challenge 4

	NEAR TERM (<5 YEARS)	MID TERM (5-10 YEARS)	LONG TERM (10-20 YEARS)
POWER ELECTRONICS CONVERSION	• Extended voltage range of (3-6kV) WBG (SiC) modules. Improved reliability of high switching frequency GaN modules (low voltage applications). • Improved high-quality UWBG substrate materials (Diamond, $Ga2O_3$, mono-crystalline GaN...). • Development of new structures (chip embedding, low inductance designs...), materials (ceramics, dielectrics, metal-matrix composites...) and assembly technologies (metal nano-particle sintering...) for WBG/UWBG packaging. • Investigation on new advanced characterization approaches for WBG/UWBG devices (high-speed spectral optical cameras, laser probing methods, etc.)	• First prototypes of UWBG devices. Devices characterization based on new test methods. • Reliability studies. Analysis of the physics of failure. • Operative WBG power modules up to 10kV (SiC).	• WBG and UWBG-based reliable power modules for optimum energy conversion in all steps of smart grids and industrial processes (low• and high-voltage range, high currents, high temperature)

	NEAR TERM (<5 YEARS)	MID TERM (5-10 YEARS)	LONG TERM (10-20 YEARS)
HTS	• Design and test of novel (cost/performance) competitive HTS nanostructured materials reaching ultimate performance through the control of the physico-chemical properties at the nanoscale. • Understanding of the vortex matter physics to approach the fundamental limits in performance, which includes determination of the optimal carrier, strain effects, frequency behavior and high magnetic field properties. • Investigation of the wire-to-device properties like thermal runaway, electromagnetic and mechanical properties, ac losses, electrical insulation, joints, geometries. • Development of computational tools to analyze HTS behavior on the device system. • Dedicated programs to strengthen joined collaborations between CSIC, institutions and industry.	• Advanced characterization and test facility for HTS superconductor modules to be integrated in real devices. • Compatibility tests and developments of low cost cryogenics. • Development of key HTS elements to couple the industrial electrification scenario with generation from renewable sources, transmission lines, power conversion devices, storage elements, motors, generators, etc.	• Development of an Interdisciplinary Thematic Platform for the management of smart power grids and new demonstrators for industrial electrification based on HTS devices (transmission/distribution lines, SFCL, SMES, AC inductive heaters, rotating machines and no-friction actuators,...).

	NEAR TERM (<5 YEARS)	MID TERM (5-10 YEARS)	LONG TERM (10-20 YEARS)
PROCESS INDUSTRY AND ELECTROCHEMISTRY	• Design of selective electrocatalysts for the direct conversion of CO_2, water and N_2 into bulk chemicals, integrating electrochemical compression. • Intensified H_2 separation/ generation in cells at > 2A•cm-2 and pressure > 5 bar. • Engineer materials and systems for industrial boilers that can switch instantly between electricity and H_2. • Development of hybrid materials (electrolytes) and interfaces to enable operation of effective electrochemical cells in the temperature range 200-450°C. • Development of materials and designs for the intensified recycling of carbon-based waste streams to yield virgin chemicals with concomitant production of power, H_2, capture CO_2 or sygnas.	• Advanced materials and cell architecture for the efficient, highly-selective separation of organics driven by electromagnetic means, also including plasma and microwave technologies. • Development of novel electrochemical devices for combined chemical conversion and CO_2 capture, integrated the use of bio-based feedstocks. • Design of selective electrocatalysts for the direct conversion of CO_2, water and N_2 into fine or specialty chemicals. • Development of electrochemical cells fully free of critical elements (noble metals and scarce metals).	• Engineering of large-scale fully-electric furnaces (>>800°C), entailing materials (ceramic and new alloys) for the furnace and heating elements, also including microwave radiation and induction methods. • Low temperature electrocatalysts for selective transformations of CO_2, water and N_2 into target molecules, also in combination with photochemistry.

ONE SLIDE SUMMARY FOR EXPERTS

Challenge

The **industrial electrification** challenge aims at replacing industrial technologies based on GHG emitting processes, by others based on electricity from renewable sources. For example, substituting natural gas furnaces for electric-powered heat pumps, electrochemical separation to replace thermally based distillation, etc. This technological transition is not straightforward and requires huge scientific efforts. This challenge is based on a deep deployment of renewable sources (solar, wind, etc.). Nevertheless, another crucial issue to solve is the transport, distribution and conversion of the energy required to reach the industrial decarbonization objectives for 2050, in an efficient, flexible and reliable way. This additional challenge will be undertaken with the development of **smart power grids**. Smart grid management based on power electronics conversion, efficient energy transmission and storage and digital technologies, will make possible (or improve) the integration of intermittent renewable sources, demand forecasting, the quality of the power, grid self-healing from power disturbance events and active participation by consumers in demand-response mechanisms.

Approach

Electrification is very promising for **industrial heating** applications, which are based on fossil fuels and are responsible for the 77% of European industrial emissions. Improvement of existing solutions (heat pumps, boilers, induction, etc.) and development of new ones (microwave, laser, electron-beam, plasma-arc, etc.) will drastically reduce CO_2 emissions. Another 23% of these emissions come directly from industrial processes, mainly in the chemical and non-metallic minerals sectors. Consequently, development of **electrochemical technologies** and electrified **materials processing** has a big potential for reducing greenhouse gas emissions. The smart power grid enabling deep electrification of industry, will be only possible with the development of key technologies: efficient transmission lines based on **high temperature superconductors**, **semiconductor power devices** for conversion systems and **digital** technologies allowing the implementation of **AI** grid management strategies

Social and economic impact

From the environmental point of view, deep industrial electrification with simultaneous implantation of renewable energy sources will drastically reduce

CO_2 emissions. The development of advanced technologies such as materials processing, electrochemistry, power semiconductors, high temperature superconductors, AI and digital control and communications, will result in the creation of economic, environmental, and social value for many industrial sectors in a sustainable manner.

Involved teams

Concerning materials processing and electrochemistry, CSIC counts on infrastructure and labs for the materials analysis and characterisation, synthesis and manufacture processes, techniques for electrochemical characterisation, reactor set-ups for catalytic testing and deposition techniques (ITQ, ICMAB, ICMS, ICN2, ICV, ICTP, INCAR, ICMM, ICP and ICB).

Regarding semiconductor power devices for electric power conversion in the grid and in final applications, CSIC has a large-scale facility (the IMB-CNM clean room) where these components have been investigated for 35 years. Superconductor materials have been investigated at CSIC (ICMAB, ICMA) and ICMAB has big experience on efficient power transmission lines. Other groups and Institutes are involved in digital and AI technologies for smart grid management.

ONE SLIDE SUMMARY FOR THE GENERAL PUBLIC

Challenge

Industry is one of the main CO_2 emitting sectors in our society. Many industrial processes are based on burning fuels and others are direct emitters of greenhouse gases. With the increasing implantation of renewable energy sources (solar, wind, etc.), these industrial processes can be replaced by others based on "clean" electricity, avoiding any emission to the atmosphere. For example, substituting natural gas furnaces in paper or food industry for electric-powered heat pumps, electrochemical separation of chemical products to replace thermally based distillation, etc. This deep "**industrial electrification**" challenge is not straightforward and requires huge scientific efforts.

This challenge is based on the deployment of renewable sources but another crucial issue to solve is the transport, distribution and conversion of the energy required to electrify the industry in an efficient, flexible and reliable way. This additional challenge will require the development of **smart power grids**. This new concept of electric distribution grid relies on efficient power conversion, transmission lines, and intelligent management of the different players (energy sources, consumers, etc.).

Approach

Industrial heating applications, based on fossil fuels, are responsible for the 77% of European industrial emissions. Heating from "clean" electric energy is the first approach for reducing them. Some existing options (heat pumps, boilers, induction, etc.) must be improved and applied to new sectors, but there are also new heating technologies requiring significant research efforts (microwave, laser, electron-beam, plasma-arc, etc.). Another 23% of CO_2 emissions come directly from industrial processes, mainly in the chemical and non-metallic minerals sectors (ammonia, lime, cement,...). Consequently, development of new **electrochemical** and **materials processing technologies** has a big potential for reducing greenhouse gas emissions. The deep electrification of industry will be only possible with the development of a **smart power grid** enabling efficient, flexible and reliable energy distribution. Smart grids will be based on key technologies: **high temperature superconductors** (transmission lines), **semiconductor power devices** (power conversion) and **digital** and communication technologies (implementation of **AI**-based grid management strategies).

Social and economic impact

From the environmental point of view, deep industrial electrification with simultaneous implantation of renewable energy sources will drastically reduce CO_2 emissions. In addition, the development of advanced technologies such as materials processing, electrochemistry, power semiconductors, high temperature superconductors and AI, will result in the creation of new economic and social possibilities.

Involved teams

Concerning materials processing and electrochemistry, CSIC counts on several infrastructure and labs for the materials analysis, synthesis and manufacture (ITQ, ICMAB, ICMS, ICN2, ICV, ICTP, INCAR, ICMM, ICP and ICB).

Regarding semiconductor power devices for electric power conversion, CSIC has a large-scale facility (the IMB-CNM clean room) where these components have been investigated for 35 years. Superconductor materials have been investigated at CSIC (ICMAB, ICMA) and ICMAB has big experience on efficient power transmission lines. Other CSIC Institutes are working on digitalisation and AI topics.

CHALLENGE 5

VALORIZATION OF BIOMASS AS ENERGY SOURCE

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1. INTRODUCTION AND GENERAL DESCRIPTION

The transport sector is the second largest energy consumer in EU being responsible for 33% of the total energy consumption and about 25% of the total greenhouse gas emissions, and relies on crude oils for 95% of its energy needs. Decarbonizing the transport sector to support climate and energy goals is recognized as a major challenge in the Energy Roadmap 2050. The development of biofuels from renewable biomass feedstocks can play an important role in this regard, supporting fuel security and the EU objective of having at least 32% of transport fuels derived from renewable sources by 2030, according to the Renewable Energy Directive 2018/2001. Plant biomass, the main source of renewable materials on Earth, is available in high amounts at very low cost (as forest, agricultural or industrial lignocellulosic wastes and cultures), and represents a potential source for the production of energy, transportation (bio)fuels and (bio)products. This chapter covers the main challenges that need to be addressed in the short, medium and long terms for using biomass as a safe, clean and efficient source of energy. Different technologies are reviewed for the production of energy from biomass, including thermochemical, biochemical and chemical processing technologies. Biomass can be burned, transformed into a fuel gas through partial combustion, into biogas through fermentation, into bioethanol through biochemical processes, into biodiesel, into a bio-oil or into a syngas from which chemicals and liquid fuels can be synthesized. The overall cost-effectiveness of biomass-to-biofuels pathways can increase significantly through the co-production of higher-added-value chemicals, and therefore, the concept of an integrated biorefinery for the production of energy, as well as chemicals, materials and commodities is also discussed. Biorefineries will definitively help maximizing resource efficiency while enhancing sustainability in the sense of the Renewable Energy Directive 2018/2001.

2. IMPACT IN BASIC SCIENCE PANORAMA AND POTENTIAL APPLICATIONS

The production of energy (and bioproducts) from biomass will profoundly influence the basic science panorama in Spain and throughout the world. Different aspects of the biomass conversion to energy, fuels and products must be addressed, from basic structural studies of biomass components to the development of efficient biomass conversion technologies through thermochemical, biochemical and chemical processes. The development of biomass conversion technologies will trigger national RTD activities focused on addressing the technical barriers, providing engineering solutions, and developing the scientific and engineering fundamentals of emerging biofuel and bioproducts industries. RTD activities in the short and medium term should focus on moving current biomass conversion technologies from concept to bench to pilot and to pre-commercial demonstration scale. RTD's long-term goal would be to accelerate the implementation of technologies by developing a deeper understanding of biomass feedstocks (including algal biomass), feedstock supply systems, and thermochemical, biochemical and chemical conversion processes. Ultimately, this knowledge can be used to develop new or improved technologies that increase the available low-cost biomass supplies, improve conversion efficiency, and reduce conversion costs while reducing carbon dioxide equivalent emissions and water use. National research groups should therefore undertake the appropriate RTD activities to develop the science and technology behind these conversion processes. The ultimate goal will be to develop the supporting technology needed to enable a fully developed, operational, and sustainable biomass-to-bioenergy value chain in Spain.

3. KEY CHALLENGING POINTS

Different technologies are used for the production of energy from biomass, including thermochemical, biochemical and chemical processing technologies. The main challenges that must be addressed in the short, medium and long term to use biomass as a safe, clean and efficient energy source are detailed in the sections below. These include improvements in the combustion, gasification, pyrolysis, and thermal liquefaction of biomass, the development of stable and robust biocatalysts with better performance for the production of bioethanol and advanced drop-in fuels from sugar fermentation, improvements in the production of biogas by anaerobic digestion of biomass (including algae and other organic residues), the development of new catalyst systems to improve the transesterification and hydrotreatment of vegetable oils for the production of biodiesel, improvements in the catalytic conversion of biomass-derived syngas into different hydrocarbon fuels through Fischer-Trops synthesis, and methanol derived fuels, as well as improvements in the production of platform chemicals from biomass, preferable via cascade-type processes. In addition, some challenges still need to be addressed for establishing fully integrated biorefinery facilities that integrate the different biochemical and chemical routes for the production of bioenergy, biofuels and bioproducts in order to improve the sustainability and the economic competitiveness of the processes. Finally, some challenges need to be addressed to produce dedicated and improved biomass feedstocks to meet the expected increasing demands for biofuels, which are also detailed below.

3.1. Thermochemical processing

Among the different ways to convert biomass into energy, fuels or chemicals, stand out thermochemical processes, namely combustion, gasification, pyrolysis and thermal liquefaction. Until now, biomass processing on a commercial scale has been used primarily for the production of heat and electricity, although the production of bio-oil is becoming more interesting nowadays, with installations of some pilot plants and commercial units in the last decade (Pang, 2019).

Combustion

Biomass combustion is commonly used to generate heat. During combustion, biomass is burned in excess of air to produce hot combustion gases, which can be directly used (drying of products) or passed through a heat exchanger to produce a hot fluid or steam. Pollutants, like nitrogen oxides, chlorides, sulfur dioxide, volatile organic compounds (VOCs) and soot, are also generated and emitted to the atmosphere. Due to regulatory and efficiency issues, the presence of these pollutants should be minimized. The combustion process is a mature technology that is in operation on a commercial scale due to its high reliability and low costs. Currently, small domestic boilers are mainly used for heat or process steam generation since they are too expensive for electricity production. The main research challenge in these small units is focused on improving thermal combustion efficiency and reducing pollutants like VOCs, soot, $PM_{2.5}$ particles, etc. In larger installations, important research is being underway on the slagging and corrosion produced by components of biomass ashes, such as sodium, potassium, chlorides, etc. The integration of biomass combustion technology with CCUS (carbon capture, utilization, and storage) technologies is also a major challenge, as they could achieve negative values for CO_2 emissions.

Gasification

Biomass gasification is a thermochemical process in which the material is transformed into a combustible gas by a series of reactions (at temperatures from 700 to 1200 °C) in the presence of a gasification agent like air, O_2, steam, CO_2 or their mixtures. The product gas consists mainly of CO, H_2, CO_2, CH_4 and other hydrocarbons. The gas composition depends on the type of biomass, type of reactor and operating conditions, but especially on the gasification agent used. When gasification is carried out with air or air/steam, the generated gas is diluted with N_2 from the air, and both the calorific value of the gas produced (4–7 MJ/Nm^3) and the energy efficiency are low. On the contrary, when oxygen, steam or oxygen/steam is used as a gasification agent, a N_2-free gas with a higher calorific value (12-28 MJ/Nm^3) is produced. However, the high cost of oxygen production is the main drawback in this case.

There are two options for biomass gasification: direct (autothermal) gasification and indirect (allothermal) gasification. Direct gasification is carried out in a single reactor with a mixture of oxygen/steam or air/steam. Part of the gas generated in the process is burned in the gasifier itself, with the air or oxygen used as a gasifying agent, to produce the heat necessary for the endothermic gasification reactions. Indirect gasification is carried out in a dual fluidized bed (DFB) gasifier consisting of two interconnected reactors (gasifier and combustor) between which a hot solid circulates. The solid fuel and usually steam, which acts as a gasifying and fluidizing agent, are fed into the gasifier where the biomass is converted into combustible gas from endothermic gasification reactions, and char. The char, together with the gasifier bed materials, are passed to the combustor where the air is introduced and the bed materials are heated by the combustion of the char. The hot materials of the combustor are passed back to the gasifier, transporting the heat necessary for the endothermic gasification reactions.

The objective of biomass gasification is to produce a gas with a composition that allows its subsequent application for the generation of heat and power, pure H_2, chemicals, natural gas synthesis or liquid fuel synthesis. Different applications may require different gas composition and purity. Syngas diluted with N_2 is used for heat/power generation meanwhile production of H_2, chemicals, natural gas synthesis or liquid fuel synthesis requires a N_2-free syngas with high purity. Obtaining a clean syngas (free of tar, particles, H_2S, NH_3) involves the use of different cleaning processes downstream of the gasifier, which consume energy and increases production costs.

Removal of tar and other minor pollutants of syngas, *in situ* of downstream the gasifier, remains the main technical challenge for the commercialization of biomass gasification technologies. Several options have been investigated to minimize the content of tar and minor pollutants in the gas produced in biomass gasification, such as the use of catalytic bed materials (limestone, dolomite, magnesite, olivine), the installation of catalytic filter candles in the gasifier freeboard, or the staged gasification (Heidenreich and Foscolo, 2015). However, more research is still needed to solve this problem obtaining better gas quality and purity, and with lower investment costs. Another challenge is to extend the gasification process to other types of organic wastes, such as refused derived fuels (RDF), sewage sludge and industrial wastes.

The use of highly integrated processes or the combination of various processes, such as a combination of biomass gasification and high-temperature electrolysis (using solar or wind energy), is currently under investigation to achieve maximum energy efficiency (Bai et al. 2015). Oxygen generated in electrolysis can be used as a gasification agent and hydrogen to produce hydrogen-rich gasification gas.

Pyrolysis

Biomass pyrolysis consists in the thermal decomposition of biomass in absence of oxygen or any other reactant due to the application of heat. During pyrolysis, solid (bio-char), liquid (bio-oil) and gaseous (bio-gas) products are generated. The fraction and composition of these products depend on biomass type and particle size, operation temperature, heating rate, pressure and residence time. Based on the operating conditions, biomass pyrolysis is usually classified into slow, intermediate, and fast pyrolysis (Varma et al. 2019). Slow pyrolysis is carried out at temperatures lower than 400 °C, with low heating rate and high gas residence time to maximize the solid fraction, bio-char, that can be used for energy generation, as an activated carbon precursor, to improve the soil quality, etc. Recently, interest in the production of organic liquid products (bio-oil) for liquid transportation fuel has increased. To maximize the yield of bio-oil, a fast heating rate, rapid quenching and appropriate operation temperatures of 400 to 650 °C are required. The bio-oil produced from biomass pyrolysis has a complex chemical composition, with high water content and oxygenated compounds. It is corrosive, immiscible with other petrochemical liquid fuel and relatively unstable. This bio-oil is mainly used for direct combustion for heat & power generation. However, a bio-oil upgrading is needed for use as liquid transportation fuel or as chemical feedstock. This can be carried out by several techniques such as solvent addition, emulsification, esterification, supercritical fluids, hydro-treating, hydro-cracking and steam reforming (Zhang et al. 2019; Varma et al. 2019; Pinheiro Pires et al. 2019). The selected process depends on the final use of the upgraded bio-oil. Hydrotreating is the most common process used for the production of liquid transportation fuels, and involves oxygen removal through hydrogenation/hydrodeoxygenation, although it is a complicated and expensive process (Michailos and Bridgwater, 2019). Further work should focus on improving bio-oil upgrading processes. To simplify the upgrading process and to improve the quality of the bio-oil, biomass pretreatment (acid leaching and torrefaction), catalytic pyrolysis, or a combination of both, have been investigated (Wigley et al. 2017; Heracleous et al. 2017). The key problem is the selection of catalysts and optimal operating conditions. The challenges associated with catalyst selectivity and stability issues and process engineering remain unsolved. In this sense, research perspectives for the coming years focus on the development of more efficient and resistant catalysts for catalytic pyrolysis. Nevertheless, biomass processing via thermal pyrolysis followed by an ulterior catalytic upgrading of the pyrolytic vapors and/or liquids to produce bio-fuels and bio-products appears to be the more profitable route from both technical and economical viewpoints.

Thermal liquefaction

Liquefaction is similar to fast pyrolysis in the way that the ultimate goal is to produce a liquid fuel. However, biomass liquefaction reactions occur in a liquid medium and usually at high pressure. The most usual process, hydrothermal liquefaction, uses water as the liquid medium. Temperature, pressure and residence time are the most important operating parameters affecting the performance and composition of the bio-oil. Application of solvents (ethanol, methanol, acetone, glycerol, phenols, ethylene glycol, etc.) and homogeneous and heterogeneous catalysts have been found to increase the yield of bio-oil and to improve its chemical composition (Pang, 2019). In general, the chemical composition of bio-oils from catalytic liquefaction of biomass is less complex than that of bio-oils from biomass pyrolysis, but in any case, upgrading of the bio-oils is still necessary.

Summarizing, biomass processing towards energy production is a well-established technology, mainly in north-European countries (Finland, Norway and Sweden). Nevertheless, some challenges remain for the complete commercialization of thermochemical processes for the conversion of biomass into energy, liquid biofuels and chemical products, mainly due to the complex nature, physical structure and chemical composition of biomass. Future research must address the main challenges: improving process performance, reducing environmental impacts, reducing capital and operation costs, and using the technologies with all type of organic wastes.

3.2. Biochemical processing

Sugar fermentation (bioethanol)

Nowadays, bioethanol is the most commonly used liquid biofuel in the world (109,891 million liters in 2019). The usual method for converting biomass into ethanol is the fermentation process, in which microorganisms (bacteria and yeasts) metabolize plant sugars to produce ethanol. Currently, most ethanol comes from corn and sugarcane crops (1G bioethanol). However, the current 1G biofuels situation (the food-versus-fuel debate) has made it imperative to develop advanced bioethanol derived from plants or plant residues that do not enter into direct competition with food markets. Lignocellulosic biomass, as woody and herbaceous crops specifically grown for bioenergy (energy crops), agricultural and woody residues, and some industrial wastes, are the most promising feedstocks for advanced bioethanol and other biofuels production. The most common biochemical conversion pathway for biofuel production is yeast fermentation to ethanol. This technology comprises the following main steps: pretreatment, hydrolysis of cellulose and hemicelluloses, sugar fermentation, separation of lignin residue and, finally, recovery and purifying the biofuel to meet fuel specifications.

The recalcitrant nature and the heterogeneous composition of lignocellulose hamper the accessibility of the sugar components to enzymes, thus limiting the hydrolysis of these materials. Technical obstacles in existing pretreatment processes include insufficient separation of cellulose and lignin (which reduces cellulose accessibility and hence the effectiveness of the hydrolysis), the formation of inhibitory by-products, the high demand of chemicals and/or energy, high costs for enzymes, and high capital costs for pre-treatment facilities (Moreno *et al.*, 2019). R&D activities are focused on converting biomass into its constituents in a market competitive and environmentally sustainable way. To advance in the development of an ideal pretreatment, it is essential to deepen into the complex physico-chemical structure of lignocellulose. It is necessary to increase our knowledge of the mechanisms of biosynthesis and assembling of the different cell wall components. Additionally, it is imperative to develop cutting-edge fractionation techniques capable of handling multi-feedstock. Reduction of the environmental impacts as well as reduction/avoidance in the use of exogenous enzymes should be pursued. Advanced analytical techniques are also needed to identify which substrate features are of particular importance to effectively pretreat cellulosic biomass and their role in determining the effectiveness of cellulose/hemicellulose enzymes.

Sugar production by enzymatic hydrolysis of pretreated lignocellulosic biomass will be an essential area for further R&D improvement by using alternative or milder pretreatment options and/or improved enzyme performance (higher conversion yields and/or lower enzyme doses or cost). Metabolic engineering strategies to improve the microbial conversion bioprocess, such as extended sugar utilization capability and robustness of microbial hosts against general stresses and toxic products, are also bottlenecks to overcome. Improving general physiology of candidate biofuel producers would allow more economically viable biofuel production, which will reduce the heavy dependence on petroleum-based fuel and contribute to slowing down global warming by providing carbon-neutral energy for the transportation sector.

Beyond ethanol

Although ethanol is the most widely produced biofuel, together with biodiesels, ethanol is not an ideal alternative fuel or blending fuel due to its low energy content (only about 70% of gasoline) and hygroscopic nature. As a result, there has been significant demand for advanced "drop-in" biofuels with better fuel properties that are compatible with the current engines and infrastructures. Good alternative transportation fuels would have similar chemical structures and properties to those in existing transportation fuels (gasoline, diesel, and jet fuels), especially in sectors like aviation, where decarbonisation options are limited. Especially for the aviation sector, it is necessary to implement advanced conversion technologies to convert sustainably produced biomass feedstocks into biofuels that are fit for the purpose of the aviation sector.

Unlike the more familiar sugar-to-ethanol fermentation route, the biological conversion pathway from sugars-to-hydrocarbons has the potential to produce less oxygenated and more energy-dense molecules, such as longer-chain alcohols like butanol and butanediol. Advanced biological routes can also convert sugars to larger hydrocarbon molecules, such as isoprenoids and fatty acids (IEA Bioenergy, 2014). These routes take advantage of previous experience in the production of bioethanol from cellulose sugars.

Hybrid conversion (biological and chemical) processes are also a promising option to transform alcohols into Jet-fuels (ATJ) (Mawhood *et al*, 2016; Gutiérrez-Antonio *et al*, 2017). ATJ processes combine biochemical production of alcohol and catalytic conversion of the alcohol into bio-jet. ATJ processes involve the production of bio-jet fuel via hydrolysis of lignocellulosic biomass into intermediate alcohols (ethanol, butanol, and fatty alcohols) and their dehydration and oligomerization. It is divided into ethanol-to-jet or butanol-to-jet technologies, depending on the alcohol involved. This bioethanol based ATJ process uses catalytic steps historically used by the petrochemical and oil refining industry. Bioethanol is dehydrated to ethylene, which is then converted via alpha-olefin oligomerization reaction into C4~C8 hydrocarbons. These hydrocarbons, separated by a selective distillation process, are reintroduced into the oligomerization process to be further converted into C6~C16 hydrocarbons in the range of jet-fuel fraction. A further step is required in optimizing the physicochemical properties through catalytic hydrogenation to achieve a high-quality biofuel for aviation.

Among other alcohols, the use of bioethanol is promising given its current production and consumption and its extensive use. Although the potential market of ethanol to be blended with gasoline seems limited for expansion, conversion to bio-jet fuel via bioethanol upgrading shows the potential of replacing existing petroleum-based aviation fuel. Bio-jet fuel is currently being developed and commercialized with various degrees of technology development readiness with various production processes used for different raw materials. However, to properly assess the technical and economic feasibility of ATJ conversion processes, it is necessary to investigate synergistic opportunities for sugar/intermediate production and process integration.

Anaerobic digestion (biogas)

Anaerobic digestion (AD) is a complex biological process in which organic raw materials are converted into 'biogas', a mixture of methane (50–75%), carbon dioxide (30–40%), and traces of other constituents, by a consortium of microorganisms that are sensitive to or completely inhibited by oxygen. The biogas produced through AD could be valorized energetically in a combined heat and power installation for the simultaneous generation of heat and electricity. It is possible to convert wastewaters from a number of industries (i.e. agro-food, beverage, alcohol distilleries, pulp and paper, etc.) into useful by-products, especially biogas by using AD (Zhang et al., 2016). AD is also used for energy conversion of different energy crops (i.e. silage maize, wheat, triticale, rye, sunflower, oilseed rape, alfalfa, etc.) in some European countries. Currently, around 18000 biogas facilities are in operation in EU, with an EU-wide installed electric capacity (IEC) of 11082 MW, and 63511 GWh of biogas produced (EBA, 2019).

Bioconversion of organic materials to methane is achieved by chemoheterotrophic, non-methanogenic, and methanogenic microorganisms with larger polymeric compounds hydrolyzed first to free sugars, alcohols, volatile fatty acids (VFAs), etc. This mixture is oxidized to acetic acid, carbon dioxide, and hydrogen, which are then converted to methane (Borja and Rincón, 2017). Depending on the temperature at which the process is carried out, biomethanation or AD of organic wastes is of three types. Biomethanation carried out in a temperature range of 45–60 °C is referred to as 'thermophilic', while that carried out in a temperature range of 20–45 °C is known as 'mesophilic', which is the most used process. The AD of organic matter at low temperatures (< 20 °C) is known as 'psychrophilic' digestion. Methane production depends not only on the operating temperature but also on other factors such as the biodegradability of the organic waste, the particle size of the waste, the pH of reactor and the presence of toxic compounds or inhibitors in the substrate such as ammonia, sulfur, some aromatic or phenolic compounds (e.g., chlorophenols), halogenated aliphatics, or heavy metals (Borja and Rincón, 2017).

Anaerobic co-digestion may improve the nutrient balance and the process performance, increasing the buffering capacity and diluting some toxics contained in a particular substrate (Fernández-Rodríguez et al., 2014). The availability of micro and macronutrients effectively alter maintenance and operation of anaerobic digesters. Micronutrients or trace elements (mainly Fe, Co, Ni) are vital for the growth and metabolism of anaerobic microorganisms, and any deficit in TE results in lower methane production. Consequently, it is essential to supplement these components to the reaction mixture, for example by a co-substrate (Rehman et al., 2019).

The development of AD technology in recent years was supported by considerable basic research that resulted in a better understanding of the microbiology and biochemistry of the process, as well as the development of many different types of bioreactors (Borja and Rincón, 2017). Improvements in reactor engineering, modelling and control practices, and molecular tools helped to better understand the process. These tools will remain some of the main challenges in the future (Rehman et al., 2019).

Using microalgae for anaerobic digestion

Microalgae are recognized as a potential source of energy due to their great adaptability, high growth rate, large accumulation of value-added compounds, etc. Microalgae and cyanobacteria can potentially be used for energy recovery through AD, although the yields obtained are highly dependent on the species and the operating conditions of growth (Zabed et al., 2020). Around 63 mL of CH_4/g volatile solids (VS) were obtained with *Dunaliella salina*, while higher methane yields of 226 and 351 mL CH_4/g VS were obtained from *Scenedesmus quadricauda* and *Chlamydomonas reinhardtii* (Fernández-Rodríguez et al., 2014, 2019a, 2019b). The low C/N ratio of microalgae and the presence of a strong cell wall hinder microalgae AD, giving low methane yields (Zabed et al., 2020). On the other hand, the use of microalgae as a co-substrate for high carbon by-products can be a very promising alternative creating a positive synergy between both co-substrates, and obtaining methane production values much higher than those obtained during microalgae AD alone (Fernández-Rodríguez et al., 2019a, 2019b). To achieve greater added-value to this type of studies, the microalgae growth in wastewaters would provide an alternative route for the removal of nutrients in wastewaters by obtaining not only nutrients removal but also a source of nitrogen-rich biomass. Improving the growth and harvesting of wastewater microalgae to be co-digested with carbon-rich co-substrates are two crucial research gaps that must be overcome for large-scale plant operation to promote the concept of sustainability and the implementation of a circular economy in the industry (Zabed et al., 2020).

3.3. Chemical processing

Transesterification and HVO for biodiesel production

Biodiesel obtained from vegetable oils or animal fats by transesterification reaction plays an essential role as a renewable biofuel. First-generation biodiesel (edible oil) is gradually being replaced by the 2nd (non-edible vegetable oil) and to a lesser extent 3rd generation (from microalgae). The European Joint Research Centre (JRC) has reported transesterification of waste oils and fats as advanced sustainable biofuels (JRC 2019). The current commercial process whereby triglycerides react with short-chain alcohol, commonly methanol, in the presence of a homogeneous alkaline catalyst has various drawbacks including saponification, isolation, purification and separation of the catalyst from the fatty acid methyl esters (FAME). Biodiesel production using acid and base solid catalysts may offer significant process advantages such as improved product separation, decreased waste, and opportunities to work in a continuous process. Solid base catalysts are preferable for the transesterification of high purity oil with low content of free fatty acids (FFA) as they are more active compared to solid acids. A solid catalyst via a continuous process has been patented by the French Institute of Petroleum (IFP) and licensed by its subsidiary Axens. However, this process is not highly commercialized since the starting vegetable oil source requires high purity. The main advantage of solid acids is that they are less sensitive to FFA and water content than their solid base analogs and hence can operate with unrefined or waste oil feedstocks. However, their application for the transesterification of oils into biodiesel is less frequently explored, in part due to their lower activity compared with base-catalyzed routes, in turn demanding higher reaction temperatures to deliver suitable conversions.

The increasing use of waste or low-grade oil sources will improve the production costs of biodiesel, but presents a challenge for catalyst design due to the presence of impurities which either requires improved purification technology or design of more robust catalysts. Solid materials capable of simultaneous esterification and transesterification under mild conditions present a future challenge for catalyst scientists. Technical advances in both materials chemistry and reactor engineering must be pursued if biodiesel is to remain a key player in the renewable energy sector during the 21st century.

Hydrotreating of vegetable oils (HVO) is an alternative process to transesterification to produce diesel from biomass. This process is a mature and flexible technology being specially interesting when using waste as raw materials.

HVO process removes the oxygen of triglycerides providing a mixture of high quality hydrocarbons, which allows blending in any desired ratio with conventional diesel. It can be coproduced in the hydrotreating plant of the current crude oil refineries. Nowadays, the main production is renewable diesel, but new catalytic systems must be developed in other to produce more efficiently as aviation and jet biofuels.

Fischer-Tropsch process and methanol derived fuels

Biomass-to-liquids (BtL) are produced by a two-step process in which biomass is converted to a syngas rich in hydrogen and carbon monoxide. After cleaning, the syngas is catalytically converted through Fischer-Tropsch (FT) synthesis into a broad range of hydrocarbon liquids. The low-temperature technology (200-220 °C, and <30 bar) provides outputs primarily for synthetic diesel and bio-kerosene production. In contrast, higher temperatures (300-350 °C) are required to obtain a mixture more compatible with gasoline. The H_2/CO ratio in synthesis gas derived from biomass is typically lower than the ratio obtained from natural gas reforming, but higher than for coal gasification. A significant concentration of CO_2 is usually present in the bio-syngas as well. Since the biomass-derived synthesis gas can contain considerable amounts of contaminants like alkali and alkaline earth species, sulfur (H_2S, COS), nitrogen (NH_3, HCN), dust, and tars a purification process of bio-syngas is usually required. The raw product should undergo a series of upgrading, such as hydrotreatment and hydrocracking, and separation processes typically used in oil refineries. Bio-syngas can also be pointed into light olefins and aromatics formation. The main challenge is to develop catalysts more robust to deactivation with higher productivity and high per-pass conversion (>75%) with higher selectivity to the targeted fraction (gasoline, jet fuel, diesel). Additional details are provided in *Challenge 7. Catalysis for the Production of Energy Resources*.

Methanol is industrially formed from syngas in the presence of a copper catalyst at 260 °C and pressures higher than 60 bar. The conversion is exothermic and very selective, transferring almost 80% of the syngas energy content to methanol. Methanol is separated from the coproduced water by distillation. Dimethyl ether (DME) can be formed by methanol dehydration in the presence of silica-alumina in a slightly exothermic reaction. DME is a clean fuel that can be stored in the liquid state at 5 bar and ambient temperature, similar to liquefied petroleum gas (LPG). DME can also be performed in a dual catalytic system in the same reactor, performing both methanol synthesis and dehydration in one-step process, syngas-to-DME. CO_2 hydrogenation to methanol at high temperature (~400 °C) is also feasible using reducible oxides as catalysts, but developing solid catalysts with better resistance to coking and the water by-product are required. In addition, it is required to develop reactors with a higher heat removal capacity (isothermal) and very high volumetric productivity. Another route via methanol intermediate that should also be considered is the Methanol-to-Gasoline (MTG) process, which was conducted for the first time by Mobil Co. in 1970 using synthetic ZSM5 zeolite. At optimized process conditions (e.g., temperature about 400 °C, and pressure 15–25 atm) the commercial plant can produce hydrocarbons in the gasoline range with 80% selectivity, and the rest of the product being mainly LPG. Finally, a general goal for all processes using bio-syngas is downscaling.

Advanced biofuels from biomass-derived sugars

Lignocellulosic biomass is generally composed of cellulose (40-50%), hemicelluloses (25-35%) and lignin (15-20%). A cost-effective fractionation process to give access to sugars and aromatics remains a challenge, although much progress has been made lately. Aqueous solutions of carbohydrates can be transformed into 2nd generation biofuels. Lignocellulosic sugars can be dehydrated to produce platform chemicals, such as 5-hydroxymethylfurfural (HMF), furfural (FUR), levulinic acid (LA) and γ-valerolactone (GVL). HMF can be transformed by hydrogenolysis into 2,5-dimethylfuran, which is a promising furanic compound to be used as a liquid transportation fuel. In addition, HMF ethers, such as 5-ethoxymethyl furfural, are considered excellent additives for diesel. The most common route for its production is the etherification of HMF with ethanol using solid acid catalysts (Melero et al. 2016). An interesting derivatization reaction of furfuryl alcohol is etherification with ethanol to form ethyl furfuryl ether, which can be blended with gasoline up to 30 wt% levels. Several methods have been proposed for obtaining liquid transportation fuels and additives from LA (Alonso et al., 2010; Mariscal et al. 2016). LA can be esterified to levulinate esters that can be blended with diesel fuel. Although these esters have poor cetane numbers, they are suitable for use as additives for gasoline and diesel transportation fuel. LA can also be converted to methyl tetrahydrofuran (MTHF) that can be blended up to 70% with gasoline without modifying current internal combustion engines. Compared with levulinic acid esters, valeric biofuels (valeric acid or ester) have a higher energy density. The conversion of LA into valeric biofuels in a one-pot approach requires bifunctional catalysts. LA can also be converted to GVL and, although it can be used as a gasoline additive, it has some limitations. GVL can also be used as an intermediate for the production of valeric and MTHF biofuels mentioned above. Finally, there are two more possibilities based on two deoxygenated molecules derived from GVL: (i) pentenoic acid can be further deoxygenated by decarboxylation and oligomerised to a mixture of C_{8+} alkanes in the range of jet fuels; and (ii) valeric acid can be deoxygenated and oligomerised via 5-nonanone to C_9 alkanes/olefins (diesel/gasoline fuels) or to a mixture of C_{18}–C_{27} alkanes (diesel fuel) upon hydrogenation.

Integrated development of catalytic cascade processes and tailored separation steps along with a lower production cost of platform products will be necessary for the future to develop competitive and sustainable processes. On the other hand, a large number of the approaches described requiere a large amount of hydrogen to remove oxygen and produce high energy density biofuels, which will have a major impact on the final cost. The transformation of carbohydrates to hydrogen using aqueous-phase reforming (APR) processes might be a good alternative (the production of hydrogen from biomass will be detailed in *Challenge 8. Hydrogen Technologies*).

3.4. Integrated biorefineries for bioenergy and bioproducts

Integrated biorefineries are the most promising way to create a new biomass-based industry for obtaining energy, fuels, chemicals and materials in a combined and sustainable manner (Liao et al., 2020), thus allowing valorizing different biological wastes with reduction of energy usage, raw materials consumption, wastes production and GHG emissions (Catalá et al., 2018). In the past two decades, research was focused on the development of biorefinery processes for the production of energy and fuels from biomass. However, due to operational and scale-up challenges, low margins and high volume production required for economic viability, great efforts were necessary to reach commercialization. Comparatively, less attention was paid to the new technologies required for the production of chemicals (and materials) from biomass, which offers advantages compared to the production of biofuels. The obtained bio-based products are more eco-friendly than the fossil-derived ones, but they are often more expensive and/or less competitive. The main challenges that the biorefinery industry must face in the next years, and recently evaluated by BBI and EERA Program EU platforms, are: i) ensure the availability and cost of sustainable biomass feedstock; ii) foster the supply of biomass feedstock to feed biorefineries; iii) improve biomass conversion and optimize efficient processing for integrated biorefineries through R&I+i; iv) further processing of intermediates (to get high added-value products); v) develop innovative bio-based products for identified market applications; and vi) improve sustainability and economic competitiveness of the processes (SIRA, 2020).

In thermo-chemical type biorefineries, biomass is mainly converted through gasification and/or pyrolysis, among other processes, into heat and power, energy vectors and intermediates (H_2, syngas, etc.), fuels for heating/power and transportation, chemicals, materials, etc. Although most academic and industry studies focused on fuels production via the biomass to liquid/gas (BTL/G) processes with syngas as primary product (i.e. Fischer-Tropsch production of diesel, bioethanol, methanol, production of methane and/or hydrogen, etc.) (Douvartzides et al., 2019), a more flexible multi-product focus is now being applied to diversify products portfolio and increase profitability. This includes production or co-production of commodities and platform chemicals (i.e. methanol), which could then be converted into other high added-value chemicals. Hence, dimethyl ether (DME), directly used as transportation fuel (Wang et al., 2016), and drop-in-biochemicals (light olefins, methyl and ethyl acetates, acetic acid, butanol, and C4+ alcohols) (Baliban et al., 2013), are the two main products envisaged to be largely developed in the next ten years.

For biochemical biorefineries, fractionation of lignocellulosic biomass into the main components (cellulose, hemicelluloses and lignin), ulterior efficient processing of the selected fraction, optimization and adequate integration of the different steps are key challenges. Up to now, cellulose has been the most employed fraction within biorefinery for bio-products generation, fuels (i.e. bioethanol) (Limayen et al., 2012), materials (i.e. cellulose fibers, microfibers and nanofibers) (Habibi et al., 2010), and chemicals (Corma et al., 2007). In the latter case, a wide range of products can be obtained using glucose derived from cellulose depolymerization via chemical and/or enzymatic hydrolysis (El-Zawawy et al., 2011). In the next years, the development of highly efficient cellulose hydrolysis processes, together with a combination of fermentative and chemical processes will allow affording several platform molecules and high-added value products useful for the chemical industry.

Glucose and glucose-enriched streams are currently treated via both aerobic and anaerobic fermentation processes to produce interesting bio-acids, such as lactic acid, succinic acid, itaconic acid, 3-hydroxypropionic acid, among others. While lactic and succinic acids are produced at industrial scale as monomers for polymer industry, the other bio-acids need further development for their scale-up. Although these bio-acids are considered important final chemicals, the production of different added-value chemicals from them is expected to be the main target to improve the competitiveness of bio-acid biorefineries in the near future (Ventura et al., 2020). Other hexoses derivatives can be obtained via chemical alkylation of glucosides (for surfactants synthesis), glucose-to-fructose isomerization, hydrogenation of glucose to sorbitol, and glucose hydrolysis/dehydration to obtain levulinic acid (see previous section). Similarly, several chemicals could be produced from hemicelluloses (C5 streams in biorefinery), such as lactic acid, furfural, xylitol and/or arabitol, and even bioethanol, among others (Gürbüz et al., 2013). Certainly, all these processes will be further developed at industrial level in the next ten years.

More importantly, pentoses and hexoses could be directly dehydrated to produce furfural and 5-hydroxymethyl furfural (Antal et al., 1991). These furanic compounds are interesting intermediates and platform molecules for the production of furan, 2-methylfuran, 2,5-dimethylfuran, furfuryl alcohol, and particularly, furan di-carboxylic acid that is used for replacing tert-phthalic acid in polymer industry (Motagamwala et al., 2018). It is expected that these products will be generally coproduced in biorefinery schemes in the next years, this including the production of aromatic compounds from furanics via Diels-Alder cyclization/dehydration process, envisaged as a new promising sugars-to-aromatics route by the EU (Biorizon Platform).

Lignin, unlike cellulose and hemicelluloses, is an aromatic polymer and offers interesting possibilities for producing chemicals, materials, and fuels that are currently obtained from fossil resources. Traditionally, most large-scale industrial processes using biomass have burned lignin to generate power. The advent of biorefineries that convert lignocellulosic biomass into liquid transportation fuels is expected to generate substantially more lignin than necessary to power operation plants, and therefore efforts are underway to transform it into value-added products (Ragauskas et al., 2006, 2014; Rinaldi et al., 2016). Thus, lignin valorization becomes imperative for biorefineries developments and profitability, and numerous EU platforms (BBI, 2020; BIORIZON PLATFORM, 2020) and projects are devoted to produce fuels, chemicals (aromatics), and materials (polymeric resins and others) by novel technology developments. However, the structural complexity, heterogeneity, and variability of the lignin polymer hinder the development of efficient conversion technologies of these materials. Indeed, and despite decades of study on lignin structure, new structural features are still being revealed, and several phenolic compounds are continually being discovered in different lignin types, thus expanding the traditional definition of lignin (del Río et al., 2020). Enhanced understanding of the biosynthesis, composition and structure of the lignin polymer remains a challenge for the full valorization of the lignocellulosic biomass.

Summarizing, although the scientific development of biorefineries is advanced, massive implementation of these models is quite slow and hampered, and their profitability must be increased. One of the problems to face and overcome is the production of low-value products such as solid or liquid fuels. In this context, an integrated approach in which bio-fuels are coproduced together with platform chemicals and other valuable chemical products (also including recovery, recycling and valorization of waste streams and effluents) is essential. Therefore, a major challenge is to provide new chemical and/or bio-chemical routes (including homogeneous, heterogeneous and enzymatic catalysis) to convert biomass into fuels and chemicals through economically viable processes. The application of cascade processes will facilitate lowering the cost of the resulting products by reducing reaction steps and separation processes, in addition to avoiding the production of wastes and GHG emissions. The biorefinery scheme will be further optimized by fully integration of different biological routes for the direct production of consumer goods.

3.5. Dedicated and improved raw materials

There is an urgent need to have dedicated biomass feedstocks for the production of biofuels and bioenergy that do not compete with those used for food and feed. Such a "food vs fuels" debate reached worldwide attention when using sugar-based or starchy feedstocks for bioethanol or vegetable oils for biodiesel production due to its socioeconomic consequences. As a response, alternative dedicated feedstocks are being explored to supply the growing demands for bioenergy. Advanced biofuels (including "cellulosic" ethanol) are still under development and have yet to reach large commercial stage. Dedicated energy crops (e.g. alfalfa, switchgrass, miscanthus), fast-growing short-rotation trees (e.g. poplar, willows, eucalyptus, paulownia) and agricultural and wood residues offer much greater potential for the biofuel industry due to its low cost and high availability. However, the economics and high capital investments for the new supply chains remain serious obstacles for 2G biofuels. For biodiesel, the search for non-edible oils from different species, as jatropha, is imperative. Algae can also be used to produce biodiesel as well as bioethanol (so-called 3G bioethanol), and microalgae are now recognized to be among the best source of biodiesel with the potential to completely replace petroleum diesel. The search for microalgae with a high rate of productivity is imperative. Plant breeding and genetic engineering techniques will help increasing the yield of these energy feedstocks. An important point to consider is the use of genetic modifications to produce feedstocks with a higher oil content (for biodiesel) or with a lignocellulose composition easier to digest (for cellulosic ethanol). Bioengineering to modify the lignin structure and/or incorporate atypical components has shown promise toward facilitating recovery and chemical transformation of lignin under biorefinery conditions. Both the mining of genetic variants in native populations of bioenergy crops and direct genetic manipulation of biosynthesis pathways will produce feedstocks with favorable properties for recovery and downstream conversion. Lignin modification in plants has been extensively investigated to reduce lignin levels or to alter its structure to facilitate pulping, improve forage digestibility, or to overcome recalcitrance of bioenergy feedstocks (Ralph et al., 2019; Mahon and Mansfield, 2019; Halpin, 2019). A main challenge will be to deepen our understanding of the chemical composition and structure of the lignin polymer and its biosynthetic pathway in different plants.

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TABLE 1—List of challenges to be addressed for Challenge 5

	NEAR TERM (< 5 YEARS)	MID TERM (5-10 YEARS)	LONG TERM (10-20 YEARS)
THERMOCHEMICAL PROCESSING	• Improve the thermal combustion efficiency and reducing pollutants as VOCs, soot, $PM_{2.5}$ particles, etc. in small units • Reduce slagging and corrosion produced by components of biomass ashes, such as sodium, potassium, chlorides, etc. • Removal of tar and other minor pollutants of syngas, in situ of downstream the gasifier, during biomass gasification	• Integrate biomass combustion technology with CCUS (carbon capture, utilization, and storage) technologies • Improve upgrading of bio-oil from pyrolysis and thermal liquefaction processes • Extend the gasification process to other types of organic wastes, such as refused derived fuels (RDF), sewage sludge and industrial wastes	• Combination of biomass gasification and high-temperature electrolysis (using solar or wind energy) to achieve maximum energy efficiency • Improve process performance, reduce environmental impacts, reduce capital and operation costs, and use the technologies with all type of organic wastes • Develop more efficient and resistant catalysts for catalytic pyrolysis
BIOCHEMICAL PROCESSING	• Increase knowledge on the mechanisms of synthesis and assembling of the different cell wall components • Understand the microbiology and biochemistry of the anaerobic digestion processes • Develop cutting-edge fractionation techniques capable to handle multi-feedstock • Improve anaerobic digestion of microalgae	• Develop more stable and robust biocatalysts, with a better performance against inhibitors and other harsh process conditions • Improve biological and chemical processes to transform alcohols into Jet-fuels • Improve the potential use of microalgae-bacteria consortia for wastewater treatment and use of the biomass generated for biogas production	• Reduce the costs of enzymatic cocktails • Identify wild or genetically engineered yeasts and bacteria capable of fermenting both hexoses and pentoses at productive yields • Develop advanced pretreatments (based on the biorefinery platform) aimed at generating added value chemicals from lignin and other components
CHEMICAL PROCESSING	• Biodiesel: develop alkaline solid catalysts for biodiesel production to improve product separation, decrease waste and allow to work in a continuous process • HVO process: develop new catalytic systems to produce more efficiently aviation and jet biofuels	• Biodiesel: develop acid solid catalysts capable of simultaneous esterification and transesterification under mild conditions	

	NEAR TERM (< 5 YEARS)	MID TERM (5-10 YEARS)	LONG TERM (10-20 YEARS)
CHEMICAL PROCESSING	• FT synthesis: develop catalysts more robust to deactivation with higher productivity and high per-pass conversion (>75%) with higher selectivity to the targeted fraction (gasoline, jet fuel, diesel) • Methanol/DME: develop catalysts that can work with high-rich CO_2 syngas, minimizing catalyst deactivation by H_2O • Advances biofuels from platform molecules: integrated development of catalytic cascade processes and adapted separation steps are required joint to cheap and widely available H_2	• Reactor upgrades for both processes: increase heat removal capacity (isothermal behaviour) joint to a very high volumetric productivity. Besides, in situ water removal is desired. • Advances biofuels from platform molecules: produce biobased platform molecules at a significantly lower cost, making their valorization to different biofuels competitive and sustainable processes.	
INTEGRATED BIOREFINERIES	• Develop strategic and logistic plans to ensure biomass feedstock supply • Improve biomass conversion and optimize efficient processing for integrated biorefineries • Further processing of intermediates to get high added-value products	• Develop innovative bio-based products for identified market applications • Full valorization of the lignin polymer from different lignocellulosic substrates • Provide new chemical and/or bio-chemical routes to convert biomass into fuels and useful chemicals through economically viable processes	• Improve sustainability and economic competitiveness of the processes • Integration of different bio• and chemical-routes for direct production of consumer goods in biorefineries • More flexible multi-product strategy to diversify products portfolio and increase biorefinery profitability
DEDICATED AND IMPROVED RAW MATERIALS		• Understand the biosynthesis, composition, structure and assembly of the plant cell wall polymers • Identify dedicated biomass feedstocks, including energy crops, lignocellulosic wastes, and algae, for biofuels and bioenergy • Produce feedstocks with improved properties through genetic engineering of bioenergy crops	

ONE SLIDE SUMMARY FOR EXPERTS

Challenge

Using lignocellulosic biomass from dedicated energy crops or wastes (agricultural, industrial, etc.), as a renewable and cost-effective source of energy and transportation fuels.

Approach

The production of energy from lignocellulosic biomass can be achieved through thermochemical, biochemical and chemical processing technologies. Biomass can be burned to produce heat and electricity, transformed into fuel gas through gasification, pyrolysis or thermal liquefaction, into biogas through anaerobic fermentation, into bioethanol through biochemical processes, into biodiesel, into a bio-oil or into a syngas from which chemicals and liquid fuels can be synthesized. The overall cost-effectiveness of biomass-to-biofuels pathways can increase significantly through the co-production of higher-added-value chemicals via cascade-type processes in the context of an integrated biorefinery.

Social and economic impact

Using lignocellulosic biomass to produce heat, electricity and transportation liquid biofuels will provide a renewable, domestically produced energy source that can be a viable alternative to fossil fuels. This will help mitigating greenhouse gas emissions, and contributing to decrease our dependency on external fossil fuel reserves. Moreover, a biofuel and/or bioproduct industry would create jobs and ensure growing energy supplies to support national and global prosperity.

Involved teams

CSIC covers the different aspects of the valorization of biomass for energy purposes, including thermochemical, biochemical and chemical processing technologies, as well as the transformation of biomass into high added-value materials/products in the context of the so-called "lignocellulosic biorefinery". Current research is spread among different CSIC institutes, including IRNAS-Seville, CIB-Madrid, ITQ-Valencia, ICP-Madrid, IG-Seville, ICB-Zaragoza, INCAR-Oviedo, LIFTEC-Zaragoza, ICMS-Seville, IATA-Valencia, among others.

ONE SLIDE SUMMARY FOR THE GENERAL PUBLIC

Challenge

Using lignocellulosic biomass as a renewable and cost-effective source of energy and transportation fuels.

Approach

The production of energy from lignocellulosic biomass can be achieved through different processing technologies. Biomass can be burned to produce heat and electricity, transformed into fuel gas via thermochemical processes, into biogas or bioethanol through biochemical processes, into biodiesel, into a bio-oil or a gas mixture (syngas) from which chemicals and liquid fuels can be synthesized. The overall cost-effectiveness of bioenergy and biofuels production from biomass can increase significantly through the co-production of higher-added-value chemicals in the context of an integrated biorefinery.

Social and economic impact

Using lignocellulosic biomass to produce heat, electricity and transportation liquid biofuels will provide a renewable, domestically produced energy source that can be a viable alternative to fossil fuels. This will help mitigating greenhouse gas emissions, and contributing to decrease our dependency on external fossil fuel reserves. Moreover, a biofuel and/or bioproduct industry would create jobs and ensure growing energy supplies to support national and global prosperity.

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CHALLENGE 6

DECARBONIZING ENERGY SECTORS ADDICTED TO CARBON: CCS AND CCU

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1. RATIONALE AND SCOPE OF THIS CHALLENGE

In order to limit global warming to below 1.5 ºC by the end of the XXI century we require zero or even negative CO_2 emissions soon after 2050 (IPCC 2018). Proposals to fully address this challenge by relying 100 % on renewables (see for example Jacobson et al. (2017)) have been severely challenged on scientific, technical and economic grounds (Clack et al. 2017). Indeed, there is quite a wide consensus (Chapter 2 of IPCC (2018)) in that a number of important industrial sectors and energy services are extremely difficult to decarbonize:

- The cement, lime, ceramics etc. manufacturing sectors emit today 1.5 $GtCO_2$/year of process emissions (about 80 % from the cement sector), that take into account only the CO_2 released from the decomposition of the mineral carbonates contained in the raw materials required to manufacture the products. Therefore, they are largely unavoidable. Switching to alternative products is a possibility for some sectors (i.e. alternative cements) but simply not possible for others (i.e. lime is a commodity that can only come from $CaCO_3$).
- The metal processing industries take a share of 5% of global CO_2 emissions. Steel manufacturing industries are highly carbon intensive (about 1.8 tCO_2/t_{steel} in the EU), because carbon-based fuels are needed as reducing agents. Decarbonisation of iron making by switching to direct reduction by H_2 or electricity is not yet possible in all applications

and at the required scales. As a result, vast flows of low heating value gases evolved from steel manufacturing processes, with a very high carbon content (i.e. ~25%CO_2 and ~25%CO in blast furnace gases), are fired unabated today.

- The chemical industries manufacturing C-containing chemicals (i.e. excluding oil, gas and refinery products to make fuels for transport) are very diverse and carbon intensive. They simply require an input of carbon atoms for their products and/or reaction pathways. The lifetime of the carbon atom in these chemicals is relatively short (i.e. less than 100 years), which means that the carbon contained in the product is re-emitted to the atmosphere as CO_2 (or as other gases with higher greenhouse gas potential).
- The renewable electricity networks of the future will still require back up power services, and/or large-scale seasonal energy storage, and/or other energy services like long distant transport of energy. Some of inherent properties of carbon-based fuels (i.e. the very high volumetric and mass energy density of hydrocarbons, as well as their low cost of transport and storage) makes them particularly suitable for these services (European Commission 2018a). Also, some forms of transport are very difficult to electrify (in particular long distance air transport and freight). Synthetic carbon-fuels, manufactured from renewable energy and renewable CO_2, can become the best solutions to address these challenges (European Commission 2018a).

It is recognized that alternative solutions to offset the emissions linked to the previous industries and services can come from the introduction of bio-energy, or by the enhancement of carbon sinks (negative emissions) to compensate for those fossil emissions that can be considered unavoidable. However, all bio-based climate mitigation options have their own limitations, arising from several economic, environmental and even geographical constrains that limit the use of biomass as a resource for energy (IPCC 2018). In such context, the use of CO_2 capture technologies for a subsequent permanent storage of the captured CO_2 (CCS), or for its use as a basis to manufacture synthetic fuels and chemicals (CCU), emerges a one of the main tools to decarbonize the previous industrial sectors and energy services. Furthermore, it is well known that CCS technologies can lead to negative emission processes (Fuss et al. 2014) when the source of carbon to the process is of biological origin (i.e. BECCS) or CO_2 is captured directly from the atmosphere (DAC).

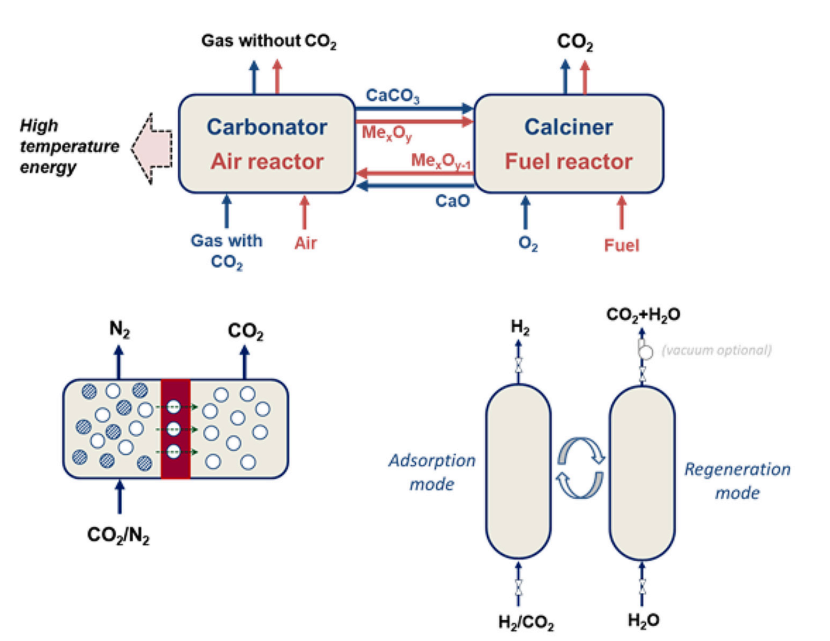
In the next three sections, we briefly introduce the scientific and technological challenges of the three main R&D topics mentioned so far: capture of CO_2 (including direct air capture), CO_2 geological storage (including uses of CO_2 in reservoirs) & processes for large scale CO_2 conversion to fuels and other chemicals. We highlight the role of several Research Centers of CSIC in these. We then list a few challenges where we think some important breakthroughs from CSIC can emerge over the next 10-20 years. A dedicated, sustained and targeted R&D effort in these fields is requested.

2. THE INTERNATIONAL R&D LANDSCAPE ON CCS AND CCU

2.1. State of the art of R&D on CO_2 capture. CSIC positioning in the field

Every CCS or CCU value chain begins with a CO_2 capture step, which deals with separating of an almost pure CO_2 stream from an energy conversion process. CO_2 capture technologies can be classified in three categories depending on where and how the key gas separation is carried out (i.e. CO_2 from a combustion flue gas, H_2 or CO_2 from fuel gases or O_2 from air to then produce rich CO_2 gases during oxy-combustion). There are mature technologies for each of these categories operating at large commercial scales. Chemical absorption with amine-based solvents or chilled ammonia is the post-combustion CO_2 capture technology having reached the largest demonstration scale. Alstom, Dow Chemical, Aker or Fluor already commercialize absorption technology using advanced amines for separating CO_2 in post-combustion applications or in natural gas and syngas purification. Regarding the separation of CO_2 from natural gas or from other synthesis gas components like H_2 and CO, larger CO_2 capture plants than for post-combustion CO_2 capture exist usually based on physical absorbents like the Selexol® and Rectisol® processes. As for O_2 production from air, cryogenic distillation is the preferred and most cost-effective technology in medium to large scale plants, with large oxy-combustion power plants constructed worldwide (30 MW_e pulverized boiler within Callide project or the Foster Wheeler 30 MW_{th} circulating fluidized boiler built at CIUDEN). Despite the maturity of these technologies, the high costs and high energy requirements associated to them pose an important barrier for their deployment. Moreover, in some of the C-based industrial sectors to be decarbonized, the implementation of these commercial systems is not feasible without incurring into deep process modifications. For these reasons, there is an active research worldwide on advanced CO_2 capture technologies with large potential of process intensification and synergy with the energy &

FIGURE 1—Emerging CO2 capture technologies (upper figure: high temperature looping solid technologies (red lines: CLC and blue lines: Ca-Looping). Bottom figures: membranes and adsorption technologies; gas mixtures chosen for comparison purposes, other mixtures could be possible).



industrial sectors mentioned before, resulting in lower CO_2 capture costs and inherently high CO_2 emissions reductions (IEAGHG 2018). The emerging technologies having undergone a substantial development in TRL in the last decade, with the highest potential of decarbonisation of C-intensive sectors are shown in Figure 1 and briefly described below, highlighting the role of CSIC in their ongoing developments.

High temperature solid looping technologies

These processes rely on reversible and fast gas-solid reactions occurring at very high temperatures between a metal oxide with O_2 (chemical looping combustion-CLC) or with CO_2 (calcium looping). In both systems, the reversible "looping" reactions at high temperatures allows for an efficient energy recovery resulting in this way in high efficiencies. CLC technology is a promising combustion technology based on the use of a metal oxide for transporting oxygen to a combustor and so avoid a direct contact between the fuel and air. This technology was initially developed for gaseous fuels, but it has been extended to solid fuels both in combustion and syngas/H_2 production applications (see reviews from (Adánez & Abad 2019; Mendiara et al. 2018; Lyngfelt et al. 2019) for more information on recent CLC progress). Gas-fueled CLC has been satisfactorily tested at 120-140 kW_{th} for combustion and reforming applications, being the operation under pressure and the need of more reactive materials the main barriers to be overcome in the development of this last application. Chemical looping applied to the combustion of solids has been demonstrated at larger scales than for gaseous fuels (TRL 6), using waste and synthetic materials as oxygen carriers. The reactivity of the oxygen carrier or the separation of the non-converted solid fuel constitute the main challenges to be overcome for improving the CO_2 capture efficiencies reached in these solid-fueled applications (Adánez et al. 2018). CSIC, and concretely the ICB, is a worldwide known leader working on the development of these chemical looping technologies as demonstrated by the number of EU projects and highly cited documents.

Calcium Looping technology relies on the reversible reaction between CO_2 and CaO to form $CaCO_3$. Ca-Looping is the emerging technology having experienced the largest development in TRL in the last decade and it has been successfully demonstrated with real flue gas and operating conditions at TRL 6-7 in the 1.7 MW_{th} pilot plant at La Pereda power station (Diego et al. 2016). The Ca-Looping technology has been reckoned by the IEA as one of the most promising emerging CO_2 capture technologies able to decarbonize the cement production industry (IEAGHG 2018), since the CaO-based material used as CO_2 sorbent can be also used as raw material for clinker production in a cement plant. Promising integration options have been assessed for integrating the Ca-Looping into cement production processes (De Lena et al. 2019) being that based on the use of an entrained flow carbonator the one with the lowest energy consumption able to separate > 90% of the CO_2 generated in the cement plant. Other highly promising Ca-Looping technologies operate in packed-bed reactors both for atmospheric and high pressure applications. Reforming of glycerine combined with a Ca-Looping system for the production of a $H_2/CO/CH_4$ gas to be converted through a FT synthesis or the decarbonization of blast furnace gas through a WGS process in the presence of a CaO-sorbent are some of the technologies being developed by ICB and INCAR-CSIC groups within different H2020 projects. CSIC (INCAR and ICB) will lead in a recently granted H2020 project the scale up to TRL 7 of these concepts in the steel industry. The INCAR-CSIC is a worldwide pioneer working in the development of the Ca-Looping technology, with ongoing patents and projects for the scaling-up of this technology for cement and steel production industries. CSIC is also active in the development of energy storage applications for the Ca-Looping and chemical looping process under European and National ongoing projects (including the use of concentrated solar power by The Institute of Materials Science of Seville (ICMS-CSIC)) and patent databases.

Membranes

The use of membranes for gas separation applications has also witnessed an impressive development in the last decade. Compared to other CO_2 separation processes, membranes are advantageous due to their compactness, simplicity of operations, low energy cost and good thermal and mechanical properties. The most widely used membranes for CO_2 separation are polymeric membranes, which are commercially used for natural gas sweetening. Nearly all commercial membranes are made from polymers due to their good scalability and low cost (Han & Ho 2018). These polymeric membranes have been studied also for CO_2 separation in CO_2/N_2 gas mixtures for post-combustion CO_2 capture applications. However, CO_2 permeability is usually limited by the low CO_2 partial pressure typical of flue gas, which hinders their application to post-combustion CO_2 capture. There is an intense effort at ICTP-CSIC for the development of polymeric membranes based on aromatic polyimides that allow reaching high gas permeability and high selectivity in CO_2/N_2 and CO_2/CH_4 mixtures (Lopez-Iglesias et al. (2018) or Aguilar-Lugo et al. (2019), among the most recent publications). Issues to be solved before the scaling-up of polymeric membranes from TRL 5 deal with the need of withstanding the aging and plasticization when applied to CO_2 separation from flue gas, as well as the higher CO_2 permeance needed to be competitive with commercial CO_2 absorption technologies. H_2 separation membranes for the purification of this gas from syngas mixtures is usually led by inorganic membranes able to sustain high temperature operation. In this case, the research is focused on developing low cost, stable and highly poison-resistant membranes able to be used within catalytic membrane reactors or as a downstream separation step. In this field of research, the ITQ-CSIC is actively working on the development of ceramic-based membranes able to achieve high H_2 permeability and selectivity at high temperatures even in the presence of H_2S (Escorihuela et al. (2018) or Montaleone et al. (2018), among the most recent publications by members of this group). Regarding the development status of H_2 separation membranes, these membranes are still at a very early stage of development (TRL 3-4) compared to the rest of membrane applications.

Finally, O_2 separation membranes have emerged as an alternative to cryogenic distillation of air, especially at small-to-medium scale where this method turns economically disadvantageous. Ceramic membranes with facilitated ion transport with perovskite and fluorite structures are the most studied membranes for this application, having reached noticeable level of development (TRL 6). The aforementioned CSIC's institutes (ITQ and ICTP) work also in the development of membranes for O_2 separation from air, especially focusing on improved selectivities and permeabilities, which are the main issues limiting their commercialization.

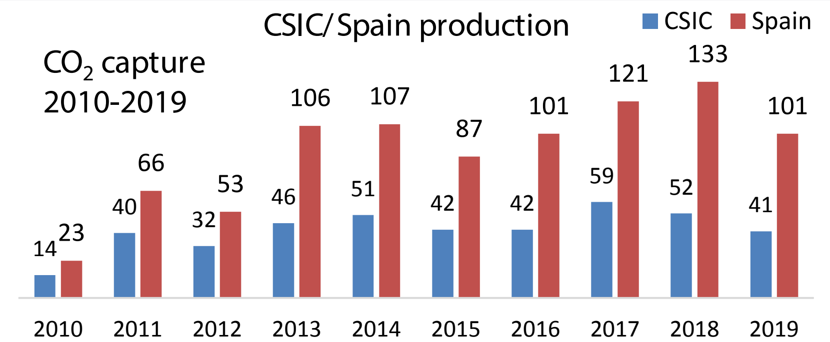
Advanced sorbent materials for CO_2 capture

As can be seen in databases of scientific publications, there is a number of high quality groups at CSIC (ICB, INCAR, ICMAB, ICMS, ICMM….) investigating advanced functional materials for CO_2 capture applications (exploring functionalised carbon materials, Metal-Organic Frameworks (MOFs), silicon-based sorbents, advanced calcium based sorbents, hydrotalcites, etc). Breakthroughs in these low TRL research could lead to substantial improvement in large-scale capture systems following gas separation strategies by pressure, vacuum or temperature swing adsorption of gases (PSA, VPSA, TSA, etc). The need to generate a highly concentrated stream of CO_2 after sorbent regeneration is a prerequisite for the application of these materials in future CO_2 capture systems.

Direct Air Capture (DAC)

A relatively new and innovative CO_2 capture technology that is at an early stage of development is capturing CO_2 directly from the air (referred to as Direct Air Capture (DAC)). Main international actors are Climeworks (that has built a plant separating 900 tCO_2/year for growing vegetables in Switzerland), Carbon Engineering (that built up in 2015 a plant separating 1 tCO_2/day), Global Thermostat, Skytree or Infinitree. Due to the very diluted CO_2 content of atmospheric air, chemical sorbents with strong binding characteristics are usually proposed for DAC purposes, like for example aqueous solutions of NaOH or KOH. DAC is an expensive and a fairly energy intensive technology today. Due to the low CO_2 contents in ambient air, extremely large flow rates of air have to be processed to collect meaningful amounts of CO_2 for climate change mitigation,

FIGURE 2–Distribution of CSIC/Spain articles reported between 2010-2019 with the term "CO_2 capture". Source: Web of Science. Clarivate Analytics. Web (May-June 2020). CSIC – URICI and BTNT (CCHS-CSIC).



which requires of vast volumes of capture equipment. Therefore, many opportunities exist for breakthrough process concepts in this field.

Regarding scientific publications in the field, CSIC participates in 47 % of total Spanish articles reported between 2010-2019 in the topic "CO_2 capture" (Figure 2), being the leader Institution at both the Spanish and European levels. It is noteworthy that Spain accounts for 17 % of total European publications in the mentioned topic and range of time *(Source: Web of Science. Clarivate Analytics. Web (May-June 2020). CSIC – URICI and BTNT (CCHS-CSIC)).*

2.2. State of the art of R&D on CO_2 storage and CSIC positioning

CO_2 storage aims at returning carbon to geologic formations. Suitable storage formations include saline aquifers, depleted oil and gas reservoirs and unmineable coal seams at depths greater than 800 m to encounter pressure and temperature conditions at which CO_2 stays in its supercritical state (Bachu, 2003). Supercritical CO_2 has a gas-like viscosity and a liquid-like density, limiting pressure build-up because of its high mobility and making storage volumetrically efficient. Yet, CO_2 is buoyant. Thus, to avoid upward CO_2 migration and achieve permanent storage, a sealing layer, known as caprock, is required (Song and Zhang, 2013). The negative public perception of the risks of CO_2 geological storage is one of the main barriers for CCS deployment. These risks can be minimized by good industrial practices already available in oil and gas operations. However, to further minimize risks, alternative storage strategies to the conventional one of injecting CO_2 in free phase have been proposed to eliminate the risk of CO_2 leakage. These strategies mainly consist in injecting CO_2 dissolved into the resident brine, leading to a sinking plume because of the higher density of CO_2-rich brine (e.g. Jain and Bryant, 2011). IDAEA-CSIC proposed a concept for storing dissolved CO_2 in the context of FP7 projects (Pool et al., 2013). Despite the lack of CO_2 leakage risk, the storage capacity is significantly reduced because CO_2 solubility into brine is just of a 4%. Therefore, storage of dissolved CO_2 may be appropriate for isolated small emitters (as some of the industrial sources mentioned in the introduction), but large emitters should inject CO_2 in free phase. A very promising option for making a benefit is to utilize the injected CO_2 as the working fluid for producing geothermal energy, leading to Carbon Capture, Utilization and Storage (CCUS) (Randolph and Saar, 2011) (Figure 3). CSIC is active in this field with an ERC grant. Industrial-scale CO_2 injection has been proven to be technically and economically feasible at several demonstration sites (Bui et al., 2018; GCCSI, 2019). The first project was Sleipner, in the Norwegian North Sea, which has been injecting CO_2 at a rate of 1 Mt/yr since 1996 (Ringrose, 2018). Other relevant projects injecting at similar rates are the Enhanced Oil Recovery (EOR) project at Weyburn, in Canada, and the In Salah Gas Project, in Algeria (Verdon et al., 2013). The whole chain of carbon capture, transport and storage was first achieved at the Quest CCS project, in Canada, storing 1 Mt/yr since late 2015. These successful experiences are paving the way to complete the challenging task of scaling up CO_2 injection rate to Gt/yr by 2040 to mitigate the climate crisis (ETP, 2017).

CO_2 plume and pressure dynamics

CO_2 injection in deep saline aquifers forms a two-phase flow in which the buoyant CO_2 tends to advance through the upper portion of the aquifer, below the caprock. The two-phase flow nature of CO_2 storage causes an almost constant pressure build-up in the long term (Vilarrasa et al., 2019). Upward CO_2 migration is impeded by the high gas entry pressure of the caprock. While most CO_2 is hydrodynamically trapped by the caprock during injection, the percentage of CO_2 that dissolves into the resident brine increases with time (Benson and Cole, 2008). CO_2-rich brine is denser than the resident brine, leading to an unstable situation in which a denser fluid is placed above a lighter fluid. As a result, gravity fingers, which enhance CO_2 dissolution (Riaz et al., 2006), are formed and their onset is inversely proportional to the vertical permeability of the storage formation (Elenius et al., 2012). If CO_2 injection is stopped, the resident brine is imbibed into the CO_2 plume due to capillarity, trapping CO_2 within the largest pores of the rock (Juanes et al., 2010). Additionally, the acidic nature of CO_2 causes a decrease in the pH of the CO_2-rich brine, promoting geochemical reactions of dissolution and precipitation of minerals and eventually trapping carbon in minerals (Zhang et al., 2009). IDAEA-CSIC has made significant contributions for the better understanding and prediction of all these processes involved in CO_2 storage.

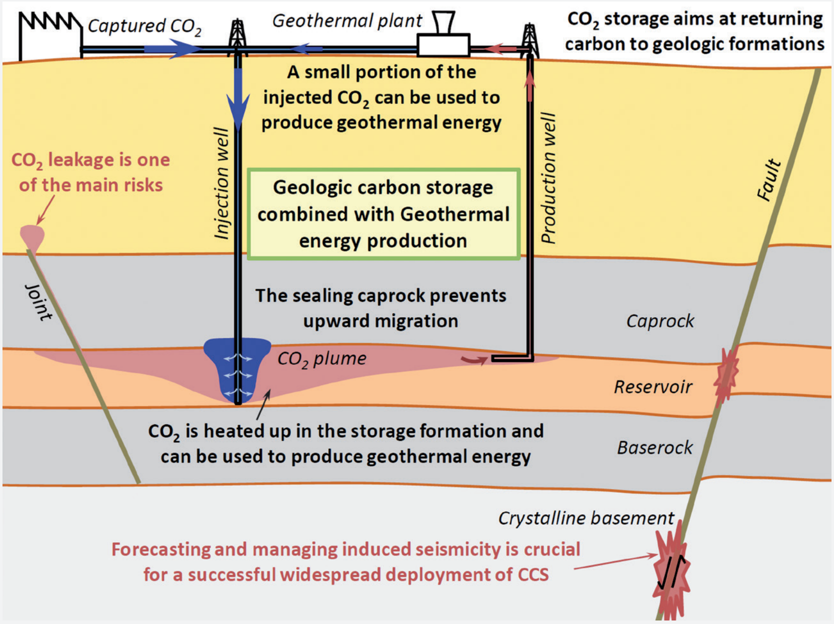
Potential for fault reactivation

No perceivable seismic event has been induced by CCS to date (Newell and Ilgen, 2019). However, public perception on any project that implies injecting a fluid in the subsurface, including CCS, is quite negative because of cases of induced seismicity related to geothermal energy, wastewater injection or seasonal gas storage. Induced earthquakes felt by the local population have led to the cancellation of projects, like the underground gas storage of Castor in Spain. Actually, such induced seismicity case may hinder the deployment of CCS in Spain. Yet, public outreach may reverse the situation if the reasons for the low induced seismicity risk of CCS, in contrast to other technologies, is explained to society. Indeed, CSIC's researchers at IDAEA have shown that geologic carbon storage can be performed without inducing large earthquakes and without CO_2 leakage provided that proper site characterization and pressure management is performed (Vilarrasa and Carrera, 2015). Currently, there is a very active research on developing methodologies to forecast induced seismicity at IDAEA-CSIC through an ERC-StG.

Monitoring, Verification and Accounting

To achieve a successful widespread deployment of CO_2 storage, effective Monitoring, Verification and Accounting (MVA) activities are required. MVA should include site characterization, CO_2 plume tracking, CO_2 injectivity, pressure, temperature, deformation and induced microseismicity monitoring, leakage detection, caprock integrity analysis and post-injection monitoring (Plasynski et al., 2011). Monitoring techniques have significantly advanced in the last years, including geophysical methods (seismic, geoelectric, magnetotelurics), tracers for monitoring CO_2 migration, capillary and dissolution trapping, fibre optic for temperature, strain and microseismicity monitoring, and well instrumentation for fluid sampling and pressure, temperature and deformation monitoring (Niemi et al., 2017). CSIC (IDAEA, ICTJA and IACT) have contributed to the development of MVA techniques. Nonetheless, reliable tools and protocols to process, analyse and interpret the huge amount of data provided by monitoring networks in real-time are still to be developed.

FIGURE 3–Schematic representation of geologic carbon storage combined with geothermal energy production, leading to Carbon Capture, Utilization and Storage (CCUS), including the main risks. The pumped CO_2 is only a very small portion of the injected CO_2 and is reinjected together with captured CO_2, allowing for both CO_2 emissions reduction and production of renewable energy.

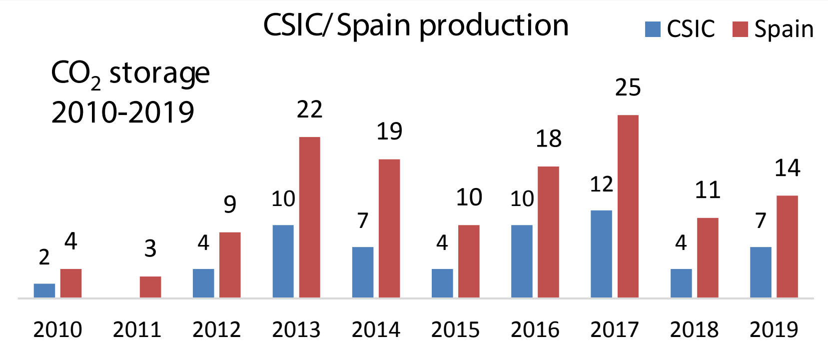


In the field of "CO_2 storage", CSIC accounts for 44% of all the Spanish scientific articles reported between 2010-2019, being clearly the leader Institution in Spain, which is the 5th ranked European country in number of publications in the mentioned topic (Figure 4). *(Source: Web of Science. Clarivate Analytics. Web (May-June 2020). CSIC – URICI and BTNT (CCHS-CSIC)).*

2.3. State of the art of R&D on CO_2 conversion and CSIC positioning

A highly appealing, but challenging alternative for reducing CO_2 emissions is using this molecule as feedstock in different chemical (or biological) transformations for producing fuels and chemicals (Artz, J. et al. 2018; Álvarez, A. et al. 2017; Ye, R-P. at al. 2019). The interest in developing these technologies up to commercial scale is on the rise and research initiatives on that direction have been promoted in several specific calls of H2020. However, being the end-product of a number of oxidation reactions, CO_2 is a very stable molecule

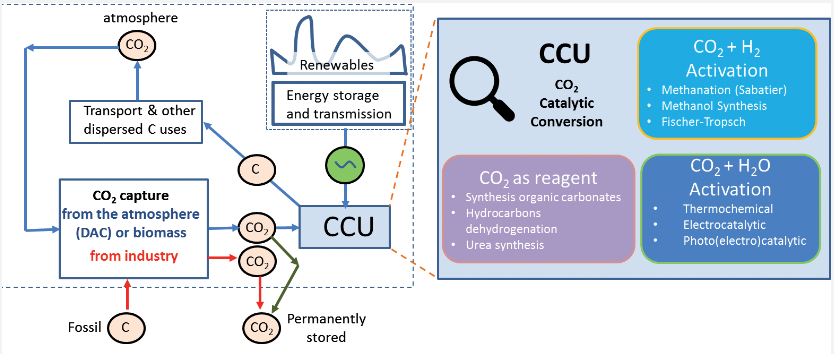
FIGURE 4–Distribution of CSIC/Spain articles reported between 2010-2019 with the term "CO_2 storage". Source: Web of Science. Clarivate Analytics. Web (May-June 2020). CSIC – URICI and BTNT (CCHS-CSIC).



with two double bonds and, therefore, its activation requires a considerable amount of energy (ΔH=279.8 kJ mol^{-1} for CO_2 splitting). Accordingly, in order to have a net effect on reducing CO_2 emissions after discounting the energy consumption of process, it is crucial to integrate renewable energy sources in the transformation of this greenhouse molecule (see Figure 5). On the other hand, the substitution of a carbon atom by a molecule of captured CO_2 in a process using fossil carbon today, translates into a reduction of a maximum of 50% of the current emissions of CO_2. For the CO_2 conversion process to be neutral or circular (i.e. with net flow of carbon to the atmosphere being zero), it is necessary that the initial CO_2 converted is also renewable (i.e. from biomass, from the atmosphere or operated in total closed loop of carbon (European Commission 2018a)).

The coupling of CO_2 conversion processes with the carbon-free energy can be indirectly provided as electricity in the so called "Power-to-Gas" scheme, or directly incorporated like in the case of "Solar Fuels" generation. Utilization of specifically developed catalysts, mainly heterogeneous, is paramount in most of these processes, although the improvement in the design of photo(electro)reactors and devices can also contribute to enhance the efficiency. Besides, it is important to keep in mind that in order to make an impact on greenhouse emissions, in addition to a high yield of energy conversion, any targeted product of CO_2 valorization should be a commodity with an important demand.

FIGURE 5–Schematic of the different routes to avoid emissions by CO_2 capture, CO_2 utilization and permanent storage of CO_2 (in geological formations or in solid products with a long lifetime). For simplicity, only the main carbon flows are represented, with "C" accounting for any form of reduced carbon or carbon product different to "CO_2". Blue arrows represent circular economy concepts (i.e. requiring capture of CO_2 from the atmosphere directly or indirectly through biomass). Red lines represent CCS near zero emission concepts when the source of carbon is fossil. Green line represents negative emission concepts. Mixed options involving CCU on industrial CO_2 sources (i.e. the red line feeding into CCU box) are not represented, because they have uncertain mitigation potential (European Commission 2018a, SAPEA report).



Accordingly, fuel production, especially for some specific niches such aviation, freight transport or back up power services, appear a clear priority by volume of demand and direct impact on emissions reduction. On the other hand, ensuring a continuous supply of high purity CO_2 is a prerequisite for all these transformations, so the existence of previous capture and separation/purification stages is implicitly assumed in the following discussion, unless otherwise is stated.

The degree of technological maturity of the different technologies varies widely, with some of them fully established at industrial scale, while others still in the initial stages of development. On the other hand, updated and realistic Life-Cycle Analysis is crucial to determine the real potential of each technology for reducing the carbon-footprint. A brief description of the most relevant routes for CO_2 transformation can be found below.

Indirect use of renewable energies for CO_2 conversion: Power-to-X

The growing availability of renewable electricity due to the extensive deployment of photovoltaic (PV) and wind farms, initially associated with governmental initiatives but now becoming the most competitive power generation technologies worldwide (see Challenge 1), inevitably causes a significant mismatch between generation and demand. This has prompted the development of strategies for using temporal energy surplus for fuels production, because overcapacity of renewable power will imply long periods of time with an excess of energy. This way of storing renewable energy has obvious advantages in terms of increasing efficiency of generation and stability of the grid, and it ushers new possibilities for the contribution of renewable sources to fuel production. The use of alkaline electrolysers for water splitting and hydrogen production is an obvious choice due to their technological maturity and the fairly high energy transformation yield (ca. 70 %), despite some economic limitations (see Challenge 8). This is the core process of the so-called Power-to-Gas route, which sometimes is generalized to Power-To-X to cover also other energy end-products, including liquid fuels.

In the context of the present challenge, this carbon-free hydrogen can be further used for CO_2 reduction to a variety of products (Artz, J. et al. 2018; Ye, R-P. at al. 2019). The most straightforward reaction is the Sabatier process for CO_2 hydrogenation to methane. This is a rather mature process with several pilot plants (E-Gas/PtG BETA of 6.3 MW at Werlte (Germany), RENOVAGAS (RTC-2014-2975-3) in Spain with CSIC participation). Currently, the main challenge of this conversion chain is the improvement of catalyst resistance to coke and sulphur. More recently, the use of novel photothermal process provides additional opportunities for solar upgrading of CO_2, as sunlight can be applied to directly drive methanation (Barrio, J. et al. 2019). Results obtained so far are encouraging, but the development of this alternative solar route is still in the lab scale (TRL 3-4).

Methanol production, which is slightly exothermic ($\Delta H = -41.2\ kJ \cdot mol^{-1}$), is more challenging, but this molecule is more valuable than methane because, being a liquid, it presents higher energy density by volume and can be further transformed to a variety of chemicals and fuels (platform molecule), such as gasoline using catalysts based on ZSM-5 zeolite (Mobil process) (Álvarez, A. et al. 2017; Zhong, J. et al. 2020). However, achieving better yields at milder conditions is still a very active research topic. Some demonstration plants for the generation of renewable methanol exist, such as that of Mitsui Chemicals and Carbon Recycling International (CRI) Inc in Iceland. On the other hand, photothermal reduction of CO_2 at atmospheric pressure has also been reported notable selectivity towards methanol, but further research is needed to develop this process (TRL 3) (Wang, L. et al 2018).

Synthesis of other oxygenated chemicals from CO_2 hydrogenation such as formic acid (potentially interesting for hydrogen storage) and, more relevantly, dimethyl ether (DME) is also attracting a great deal of interest. Direct transformation of CO_2 to DME involves two reactions, methanol synthesis and its subsequent dehydration, which requires bifunctional catalysts comprising both metallic and acidic centres (Álvarez, A. et al. 2017). This is a rather mature process but enhanced resistance of the catalyst to water generated as by-product and coke formation is required.

Finally, the well-known Fischer-Tropsch (FT) route to synthetic fuels can be also fed with CO_2 and H_2 blends, instead of syngas. In this case, the FT process is expected to proceed via reverse water−gas shift (rWGS) reaction and consecutive CO hydrogenation to hydrocarbons in a wide range of chain length (Zhu, W. 2019). As for traditional FT processes (from syngas), there is also the possibility to directly produce specific synthetic liquid fuels (e.g., gasoline) from CO_2/H_2 in a single-step process by using multifunctional catalysts combining an Fe-based FT component with an acidic co-catalyst (e.g., zeolite). This one-step process avoids the wide distribution of hydrocarbons typical of conventional FT technologies requiring an additional upgrading stage. Selectively producing hydrocarbons in the jet fuel range instead of gasoline is desirable albeit more challenging. ITQ-CSIC is well positioned in this area by leading a current H2020 project for the direct hydrogenation of CO_2 to aviation fuel. Furthermore, CO_2 reduction to light olefins (C_2-C_4) and BTX aromatics is also possible with specific multifunctional catalyst (Wang, S. et al. 2020; Cui, X. et al. 2019; Ni, Y. et al. 2018). FT is industrially used for CO_2 conversion (plant of Shell in Qatar) but there exists a significant interest in further reducing the carbon footprint by increasing the energy efficiency and the share of renewables.

Dry reforming of methane is an important process for CO_2 activation leading to the production of syngas, which can be further processed by conventional Fischer-Tropsch into synthetic fuel (Artz,J. et al. 2018) (see also Challenge 7). Recently, the successful use of chemical looping scheme for methane dry reforming has resulted in improved resistance against coke deposition and better opportunities for solarisation, although additional improvements are pursued (Sastre et al. 2019). Electrochemical processes, ideally powered by renewables, provide a more direct route for CO_2 conversion, without using externally produced hydrogen. At present, electrocatalysts face several challenges because they operate with high overpotentials, low faradaic efficiency due to the competition of water decomposition with CO_2 splitting, low current densities and they deactivate over time. Electrodes of Cu have frequently been used for this process because they can reduce CO_2 to hydrocarbons (i.e. methane, ethylene) with reasonable faradaic efficiency. Depending on the catalyst methanol, formic acid and CO are other possible products of the electrochemical reduction of CO_2, but in general with limited efficiency (Kondratenko, E.V. et al. 2013).

High temperature solid state devices have been proposed for the direct electrochemical conversion of CO_2 into different products such as methane, syngas or even specific hydrocarbons fractions, when combined with additional thermal catalysts. Operating at high temperature can improve the kinetics and decrease electric energy consumption, but better electrocatalysts are required and this has prompted a very active research in this field (Vøllestad, E. et al. 2019).

Direct routes for CO_2 conversion using solar energy: Solar Fuels
Photocatalytic reduction of CO_2 is a very challenging but highly rewarding route for converting that molecule into fuels. This process is frequently referred to as artificial photosynthesis (Herron, J. A et al. 2015; Fresno, F. et al. 2019). However, this denomination can be misleading because in contrast with natural photosynthesis, it leads to the production of much simpler molecules than glucose (e.g. CH_4 or CH_3OH) and requires anaerobic conditions. Currently, research efforts are mainly focused on the development of more active and selective catalysts, which can boost the current rates of transformation (generally in the range on $\mu mol \cdot g^{-1} \cdot h^{-1}$) and increase the selectivity to molecules with higher energy density than CO, which is usually the majority product. Due to the current limitation in the energy yield (apparent quantum yield <1%), these technologies are still mainly at the lab scale (TRL 3-4).

Alternatively, light and electricity can be jointly applied for activation of CO_2 in photoelectrochemical processes, which implies the use of illuminated semiconductor electrodes (Zhao, G. et al. 2017). This route can yield a variety of products, including methanol or CO, but, as in the case of electrocatalytic processes, controlling selectivity and stability while reducing overpotentials are required for further development of these devices from lab scale (TRL 3-4).

Recently, thermochemical cycles fed with CO_2 and H_2O have led to solar to fuel energy conversion exceeding 5 % (Marxer, D. et al. 2017). The product of this process is syngas, which requires further conversion by Fischer-Tropsch or other route for achieving a liquid fuel such as kerosene. Despite the technical complexity of this technology, which needs large facilities and extreme conditions of temperature, demonstration plants of considerable size (250 kW) have confirmed the feasibility of this process under real concentrating solar light (TRL 5-6). However, research on materials operating at milder conditions is very active worldwide, in order to reduce the severity of the conditions and widen the window of operation.

Biological transformations using selected or genetically manipulated synthetic organisms, mainly microalgae, have been also proposed and assayed at realistic conditions using specifically designed photobioreactors (TRL 6-7). In contrast with other technologies, these biological systems do not require CO_2 purification, and efficiency in the utilization of solar light is higher than for photochemical processes. However, recovering the biomass from the aqueous media and the subsequent extraction of the chemical (e.g. triglycerides, pigments...) from the cells is energy demanding and may compromise the capacity of this route for CO_2 reduction.

Processes for incorporating CO_2 in chemicals and polymers

Currently, in addition to the mature process for urea production (180 Mt/yr in 2016), one of the main interests of the utilization of CO_2 in the chemical industry is the synthesis of organic carbonates (Artz, J. et al. 2018). Dimethyl carbonate is widely used in chemical electronic and fuel industries (current production 90 kt/yr). The conventional industrial process uses extremely toxic phosgene for the carbonylation of methanol, but alternative routes exist using CO_2. Although direct reaction with methanol is limited by equilibrium, cyclic carbonates can be alternatively obtained by reaction of CO_2 with the corresponding epoxide using ammonium halide-based catalysts. In this way, ethylene oxide can be converted first into diethyl carbonate, and then into diphenyl carbonate by transesterification with phenol (Asahi process). This route can be used for the subsequent synthesis of Bisphenol A based polycarbonate, which has been already implemented in several commercial plants. On the other hand, production of poly(ether carbonate) polyols from propylene oxide and CO_2 is also feasible in a process developed by Covestro. Other reactions, such as those involving CO_2 and olefins have been also investigated for some niche chemical production.

From a different perspective, CO_2 can be also used as mild oxidant for the oxidative dehydrogenation of alkanes and alkyl aromatics (CO_2-ODH) to yield the corresponding olefins and olefinic aromatics (e.g. styrene), respectively. In comparison to conventional ODH using O_2 as oxidant, the CO_2-ODH process avoids overoxidation and reduces coking.

3. SPECIFIC R&D STRATEGIC CHALLENGES

What follows is a list of themes or research topics that, in the opinion of the authors, can make a real impact in solving some of the previous global challenges. The order of the challenges reflects today's participation of CSIC in these challenges.

- Development of new generation of catalysts for CO_2 conversion with enhanced performance. Most of the catalysts employed in the different routes for CO_2 hydrogenation are fairly efficient, but additional advantages can be achieved by improving durability, selectivity and reducing costs of these functional materials. However, in the field of solar fuels the design of catalysts with enhanced performance (particularly photo/(electro)catalyst), with capacity to significantly improve the energy conversion yield (expected to be ca. 15% for industrial applications), will be critical for these technologies to progress towards a future commercial deployment in the medium term. These aspects are expected to continue to be hot topics of scientific interest in the following years.
- Integration of processes for promoting energy efficiency and the search of positive synergies between different conversion routes. Improving energy efficiency is one of the pillars of reducing the carbon footprint but it has been scarcely considered for most of the processes of CO_2, although opportunities for a better use of energy are expected to arise from a global design of the reactors with fully integration of heat recovery components. This is particularly important when considering the complete process, including the stages of CO_2 separation and purification. In addition, use of renewables, including solar heating, for powering some stages of the process in Power-to-X routes can be feasible. More importantly, integration of different routes of CO_2 transformation has been scarcely explored because usually different technologies have been considered as competing alternatives. However, important synergies may arise from considering the smart coupling of different value chains.
- Development of advanced CO_2 capture processes. Separating a highly concentrated stream of CO_2 from flue gases or low quality fuel gases is known to be a costly and energy consuming step for today's industrial sources of CO_2. It is necessary to develop advanced CO_2 capture technologies for those industrial sectors that cannot be decarbonized, and to allow carbon negative schemes by direct CO_2 capture from air or

in future biomass-based processes. This will involve new reactor concepts (high temperature looping systems, advanced membranes and sorbents, etc.) using superior functional materials for gas separation at large scale. Also critical is to investigate smart integration of processes that can exploit synergies between gas separation and CO_2 conversion steps to minimise carbon footprints and overall process cost. This last point requires multiscale and multidisciplinary system/process modeling efforts that are gaining increasing importance to connect several fields and disciplines of the overall Energy challenge.

- Upscale CO_2 storage to significantly reduce CO_2 emissions. Individual sites storing CO_2 in the order of 1 Mt/yr have successfully demonstrated the feasibility of safely storing CO_2 deep underground. However, the annual injection rate should be scaled up globally to the Gt scale within the next decades to permit cutting down CO_2 emissions according to the climate goals of the Paris Agreement. Dynamic pressure limits at the basin scale should be better understood to maintain the caprock sealing capacity, avoid CO_2 leakage and prevent inducing unacceptably large earthquakes.

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TABLE 1—List of challenges to be addressed for the Challenge 6

	NEAR TERM (< 5 YEARS)	MID TERM (5-10 YEARS)	LONG TERM (10-20 YEARS)
CO_2 CAPTURE	• Develop advanced CO_2 sorbents, oxygen carriers and CO_2, H_2 or O_2 membrane materials • Develop optimum capture technologies for industrial sectors (non-power)	• Scale up reactors of new capture technologies to TRL 6-7 • Pilot testing of biomass-based processes with CO_2 capture	• Direct CO_2 capture from air • TRL 7 demonstration of negative CO_2 emission concepts
CO_2 UTILISATION	• Optimization and extensive deployment of Power-To-Gas and Power-To-Liquids technologies • Develop more efficient catalysts for challenging direct CO_2 conversion processes with the integration of renewables	• Scale-up of the most promising and mature solar fuels technologies • Demonstration plants for the coupling of CO_2 capture, specially form air, and conversion	• Achieving commercially viable yields in photoactivated and other promising advanced technologies • Widening the integration degree of conversion technologies in new energy schemes • Launching of new emerging concepts for CO_2 transformation
CO_2 STORAGE	• Increase the number of Mt-scale storage projects • Develop pressure management protocols for Gt-scale storage	• Implement pilot tests of BECCS and CCS combined with geothermal energy production • Enable the production of blue hydrogen at scale	• Scale up CO_2 storage, having multiple Mt/yr injection wells within the same storage formation • Achieve deep decarbonization of the hard-to-abate industry
CROSSCUTTING	• Smart process simulation of wider systems (i.e. integrating CO_2 capture and utilisation technologies, incorporating renewables)		

ONE SLIDE SUMMARY FOR THE GENERAL PUBLIC

Challenge

Avoid emissions of CO_2 to the atmosphere from industrial sectors that must produce CO_2 to exist (example: cement, steel, others), or that need to burn fuels with carbon (aeroplanes, freight, etc.) or that simply need carbon to manufacture chemicals that then decompose and produce CO_2 (fertilizers, polymers, etc).

Approach

Capturing the CO_2 from the flue gas source or from the atmosphere, purifying it and then either storing it permanently underground (to completely avoid its emission to the atmosphere) or re-using it (to partially reduce or delay emissions) in different chemical processes, mainly for fuel production.

Social and economic impact

These technologies will be needed to reach 100% decarbonisation targets to combat climate change. They can allow for negative emissions systems, that is, reducing the CO_2 concentration from the atmosphere, when biomass is used as a fuel in the primary industry.

Involved teams

CSIC has several teams investigating capture of CO_2, utilisation or conversion into products and fewer experts on CO_2 permanent storage.

CHALLENGE 7

CATALYSIS FOR INDUSTRIAL PRODUCTION AND OF ENERGY RESOURCES

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1. FOREWORD

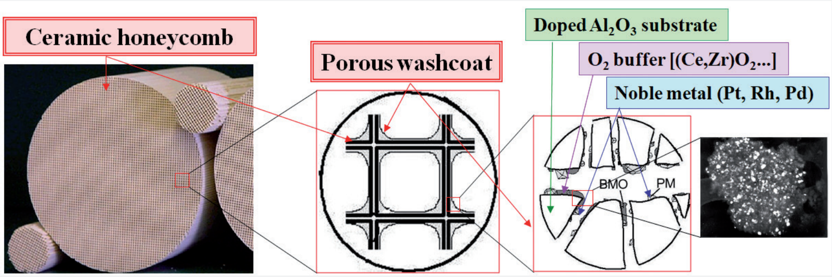
Catalysis is a key enabling technology for various challenges in the Energy Area; is also relevant for chemicals production, environment protection, selective synthesis, sensing and other key subjects. To quote a document from the European Cluster of Catalysis (ERIC, 2016):

> "Catalysis and catalytic processes account directly or indirectly for about 20-30 % of world GDP."... "Of the 50 largest volume chemicals currently produced, 30 are produced via catalytic routes... and account for more than 20 billion tons of CO_2 emitted yearly to the atmosphere... Technical improvements in catalyst processes could reduce energy intensity for these products by 20% to 40% by 2050."

There are also specific issues common to many fields of general catalysis:

1. Many catalysts have complex structures, not only at molecular level, as in enzymes and homogeneous catalysts, but also in morphology (Figure 1). Catalytic active species in solids may need to contact other phases (maybe at specific surface planes), to exist as particles of narrow size range, etc. It is thus important to master catalyst synthesis methods. Besides, some catalysts require precious or rare metals, or hard to produce ligands; they should be manufacturable more easily, with less cost and/or in less steps.

FIGURE 1–Typical three-way catalyst for exhaust gas treatment in gasoline cars. Source: composed by J.C. Conesa using images from very different sources.



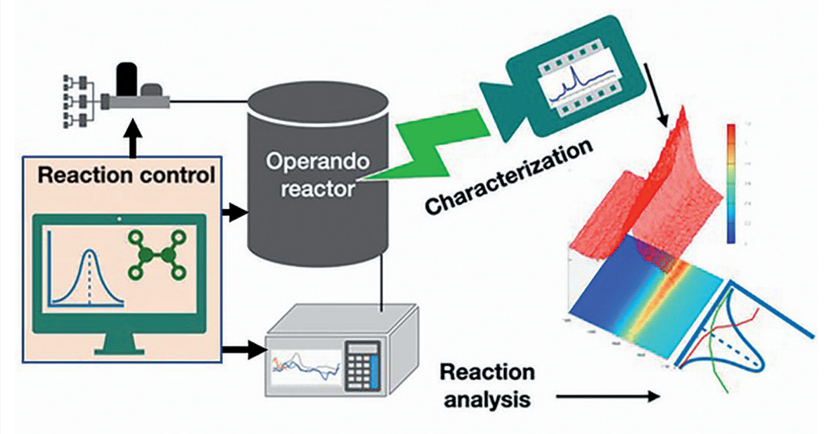
2. Catalyst modelling is key to identify reaction mechanisms and catalyst active centers. Reliable predictions of catalysts behaviour need using multiscale approaches (Bruix, 2019) that combine calculations of geometric and electronic structure, reaction barriers, molecular dynamics (MD) and atomic scale microkinetic modelling, to end with macroscopic transport models and classical reaction engineering. The different scales may be computed separately to higher or lower accuracy and then combined strongly or weakly.

   Electronic structure calculations study bond breaking/forming steps and activation energies. MD can use atomistic potentials, semiempirical or DFT systems. Mean field or Monte Carlo methods can be used in larger scales. Powerful hardware and software tools allow realistic catalyst models at working conditions of P, T and fluids. Machine learning (Kitchin, 2018) and AI techniques are used today to design and prepare better catalysts (even using robotic systems) and can be combined with multiscale modeling frameworks.

   Many CSIC groups use computational tools for catalysts modeling. Main ones work at ICP, ITQ, ICMM or IIQ; others working in materials modeling could adapt their tasks. Parallel supercomputers are needed, like those available in RES and PRACE networks.

3. Studying the state of a working catalyst may need in situ techniques. Many of them can be used: XRD, IR, Raman, UV-Vis-NIR, NMR, EPR, XPS, synchrotron radiation-based spectroscopies... Catalysis studies also

FIGURE 2—The operando methodology. Source: made ex novo by Miguel A. Bañares.



require relating performance and structure. Both can be combined using the operando concept (Bañares, 2005) (Figure 2), where reactants and products are measured to check that the reaction takes place like in the catalytic reactor; multimodal reaction cells compatible with the probes used and working at the desired conditions (T, P, gas/liquid flows, etc.) can be designed. Catalysis may also require characterizing both catalyst and catalytic reactions with time- and space-resolution. CSIC institutes working in this line are mainly ICP and ITQ; if CSIC wants to foster research lines on catalysis it might be convenient to promote in other institutes the use of *operando* equipment.

4. New types of catalytic reactors need to be engineered. Intensification implies using multiple very narrow channels in parallel; membrane reactors allow separation of products as they are formed; photocatalysis needs clever handling of photon flow; fuel cells and electrolyzers, like photoelectrochemistry, require well-designed gas diffusion electrodes; other reactor designs may be needed to allow greener processes, etc.

Another important aspect is whether concentrated or distributed technologies should be preferred, aiming at reducing CO_2 emissions. This is subject of a recent review (Smith, 2020) focused on NH_3 synthesis, but can be applied to many processes, even to non-catalytic ones.

All these aspects are relevant for any catalytic processes, including energy-related ones.

2. CATALYSIS FOR A SUSTAINABLE INDUSTRIAL PRODUCTION

2.1. Catalysis for industrial production with lower energy demand and higher atom efficiency

Catalysis is one key technology driving a Sustainable Chemistry; it makes possible improving energy efficiency, using renewable feedstocks and reducing waste (Anastas, 1998). Concerning energy, catalysis enables producing clean fuels and using renewable resources (e.g. bioethanol), thus decreasing the overall carbon footprint. It also improves energy efficiency of chemical processes with disruptive techniques based in new catalytic routes.

Industrial chemical processes can be of two types: with high volume but low added value of the product (commodities, chemical intermediates, platform molecules) and with (very) small volume and high added value (speciality chemicals, pharma, etc.). The energy balance of a chemical reaction is fixed, but the energy input of its industrial process depends on the conditioning of its reactants (T, P) and on the need of separation and purification of products, which may cause more than 90% of the overall cost.

Impact in basic science panorama and potential applications. Key challenging points

Two catalyst properties are key to improve the energy efficiency:

- a) high activity allowing process operation at milder conditions (low P and/or T) or high productivity at given reaction conditions (reducing the energy input per unit product).
- b) high selectivity to the targeted product, reducing separation/ purification costs.

Better energy efficiency may come also via process intensification, integrating chemical reaction and process physical steps, and optimizing process and reactor design. This will require developing or morphologically adapting catalysts to new environments and operational regimes: high per-pass conversion or productivity, passing from overall endothermic to exothermic systems or vice versa, etc.

Another main role of catalysis in chemistry concerns atom efficiency (Sheldon, 2000). Catalysts allow substituting classical organic syntheses which require stoichiometric amounts of reagents and/or may reduce the number of steps needed. Selectivity is a key catalytic property, to keep most reactant atoms in the final product. Novel selective catalysts and improved selectivity of current ones are key research goals in this field.

Homogeneous catalysis with its high selectivity is a good example. Thus, aminations inserting NH_3 in simple organic molecules containing C-C double bonds, alcohol or carbonyl groups can proceed now without deactivation and high yield using recent metal complexes; this provides key compounds for the pharma industry.

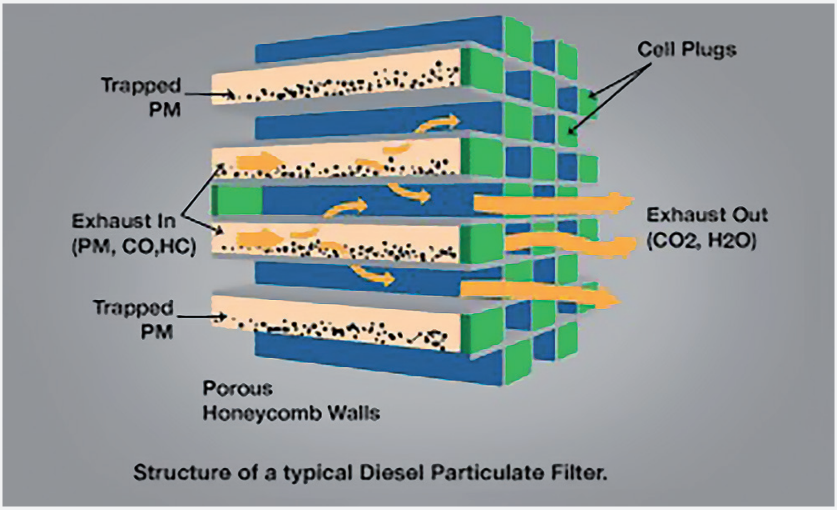
The best example of these principles is given by enzymatic catalysis. It conforms most principles of green chemistry (Graedel, 2006), e.g. no. 6 stating that "Energy requirements should be recognized for their environmental and economic impacts, and should be minimized". Most enzyme-catalyzed reactions occur in aqueous media at mild temperature (T, from now on), e.g.<60ºC, lowering energy needs, though product separation may be difficult.

Enzyme-catalyzed processes can be made in batch reactors. Several enzymatic processes may operate under similar T and pressure (P, from now on) conditions, allowing integration of multiple transformations into economically attractive cascade processes. Such processes can also have very high selectivity, alleviating the need of by-product separation. Besides, many enzyme catalysts are obtained from easily available renewable resources, and are biodegradable and (except for some metalloenzymes) non-toxic. They do not need functional group activation, protection and deprotection steps, generating thus less waste than other methodologies. Biotechnology advances make now feasible to optimize and adapt enzymes to a predefined process. Protein engineering, especially directed evolution, can improve enzymes to design sustainable processes with less generation of residues. This strategy was already used successfully e.g. in industrial synthesis of pharmaceuticals.

2.2. Air depollution in energy-intensive industries

The measures taken by industrialised countries after signing the 1997 Kyoto Protocol have led to reduction in emissions of greenhouse gases and toxic pollutants in transport, electricity generation and chemical industry. Spain adopted such measures (improving fuels, substituting fossil fuels by other energies) establishing end-of-pipe treatments, fixing pollutants by ad- or ab-sorption, or transforming them into harmless substances via catalytic or

FIGURE 3–Honeycomb system treating gases and soot from industrial Diesel motors. Source: http://urbanemissions.blogspot.com/2015/12/what-is-diesel-particle-filter-dpf.html.



non-catalytic processes. This has originated a series of documents (http://www.prtr-es.es/documentos/documentos-mejores-tecnicas-disponibles).

Impact in basic science panorama and potential applications

Several mature technologies exist, at TRL9, to clean gases from NOx and SO_2 in combustion plants: low NOx burners, flue gas recirculation, selective non-catalytic (SNCR) or catalytic (SCR) reduction, etc.; the latter shows good efficiency in high dust systems working at 300-450 ºC. New trends try to improve stability against K+ present in ashes, especially with biomass fuels (Schill, 2018), and to lower the catalyst working T below 200ºC to use the SCR system in tail-gas, avoiding problems due to the presence of SO_2 and ashes in the catalyst. Other techniques are proposed for SO_2 elimination: using low-sulphur fuels, injecting sorbents in the boiler and wet desulphurization using aqueous solutions to capture acid compounds. This requires improving cost reduction and reusing/recycling the products resulting from sorption. Achieving TRL7-9 needs replacing noble metals by less costly transition metal oxides in catalysts burning VOCs.

N_2O emissions during fertilizers production must be avoided, as they contribute to the greenhouse effect. Several TRL6-8 options under development are being considered.

Key challenging points

Cleaner processes, new catalysts and more efficient, durable and cheaper absorbents are needed to further reduce emissions. Activation of materials by photons or μw to avoid heating all the gas mass or structures like wall-flow monoliths (Figure 3) are some options. New methods of catalyst manufacturing must be developed here, both for the synthesis of nanoparticles and for the structuring of solids, e.g. using 3D additive manufacturing.

2.3. Catalytic processes directly driven by electricity and electromagnetism

Impact in basic science panorama and potential applications.

Key challenging points

Some catalytic processes (besides electrochemical ones) can be driven by electricity without transforming it to heat: microwave (MW) activated catalysis, plasma-catalysis and use of magnetic fields are emerging alternatives likely to spread over the next years.

MW is used to process materials, biomass or wastes; also for catalytic reactions (Martín, 2018), due to high energy delivering rates, ability to provide uniform or localized activation, or reduction of process time and energy use (30-50%). MW can also provide better control of catalytic selectivity. Current commercial use of MW in catalysis, biomass processing or materials synthesis is still scarce, as the interaction between MW and solids/liquids or reactants/catalysts is not yet understood. Problems as measuring hot spots T or the need to improve reactors design also hinder the progress of this technology.

Plasma can be used to induce gas reactions at ambient conditions and short/zero response times. They may replace energy demanding processes, reducing their CO_2 footprint, e.g. in Haber-Bosch NH_3 synthesis (responsible for 1.7% of CO_2 emissions). Both MW and direct DC/AC activation modes can induce atmospheric plasmas for gas phase processes (Snoeckx, 2017). Using plasmas at high TRLs faces limitations to treat large gas volumes, have high energy costs and, in some cases, also difficulties to control selectivity.

Magnetic fields generated by AC currents can efficiently heat magnetic nanomaterials coupled with catalysts .in microreactors and flow systems. This technology was first used in 2008 for the oxidation of alcohols, using gold-doped magnetic nanoparticles as catalysts. It has been tested recently in biocatalysis to increase and regulate the catalytic activity of linked enzymes (Hotzyme, 2019), and in the degradation of organic pollutants.

A challenge common to all these emerging techniques is improving efficiency at large scale; i.e. move the technology to higher TRL values. This has specific limitations:

MW-induced catalytic processes: i) Scaling up reactors while compensating the small penetration of MW; ii) Improved reactor designs (operation modes, feedback systems, automatism); iii) Catalyst design adjusting each material to its capacity to absorb MW.

Plasma-catalysis: i) Improving reaction yield (better electrode materials, alternatives for gas handling systems); ii) Increasing energy efficiency (vortex handling of gases, using gliding arcs, etc.); iii) Better selectivity via formulation of plasma-specific catalysts.

Catalysis assisted by magnetic fields: i) Improving the energy efficiency for large scale processes; ii) New catalyst formulations to enhance activity and reduce costs.

New promising research lines can thus arise using renewable electricity. MW may find use in pyrolysis or reactions valorizing biobased chemicals, polymers and waste in medium/large scales. Plasma-catalysis may expand to treat small gas volumes, e.g. for n-situ H_2 production from organics or NH_3 or in on-board reactors for cars or ships. Magnetic field activation can be used in niche applications: biocatalysis or sanitization.

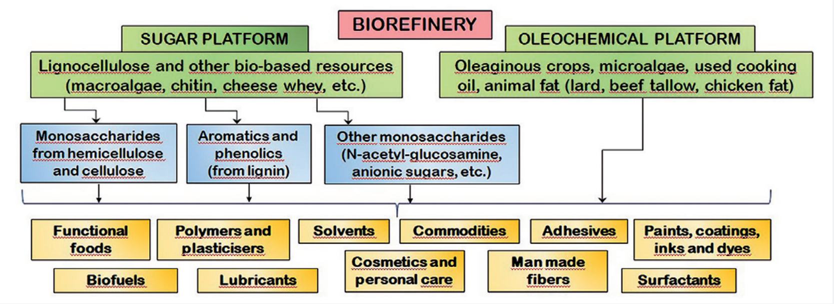
3. CATALYSIS FOR THE USE OF BIOMASS

Impact in basic science panorama and potential applications.

In last years industrialised countries have turned to biomass as a renewable carbon source for producing food, fuels, materials and chemicals in the so-called biorefineries (Figure 4), fully aligning with the European Bioeconomy and Circular Economy Strategies and the longer-term Objective of Going Carbon Neutral by 2050 announced by EU.

The second-generation biofuels sector (those not competing with food) is well established in Europe. However, the bio-based chemicals sector, even being already a reality in EU with annual turnover of 9.17 M€, still represents only 3 % of EU chemical industry according to a report issued by the European Joint Research Centre (JRC) (Spekreijse, 2019). Some sectors (coatings, paints, inks, etc.) are mature; others (platform chemicals, plastics, adhesives, lubricants, etc.) have high growing potential.

FIGURE 4—The biorefinery concept. Source: made ex novo by F. Plou, with additions and rearrangements by M.A. Centeno and M. López Granados.



Processes to transform biomass to products can be fermentative, enzymatic or chemical. The first one is out of the scope of this text as it cannot conduct many needed reactions feasible only with chemo- and biocatalysts. Chemocatalysis is robust, productive and suited for lower cost chemicals; enzymes, with better selectivity, operate in milder conditions (Sheldon, 2018). Combination of both types of catalysts (combocatalysis) in a single cascade process is a promising option which is currently at early stages of research.

Key challenging points

Catalysis in production of biofuels and renewable chemicals from biomass

The main research challenge in chemo- and biocatalysis is to produce cost-effective bio-based products. Processes must be efficient, robust (coping with impurities or water, leaching, thermal changes, etc.), durable, flexible to adapt to different biomass types and to meet the green chemistry rules; separation/purification steps must be integrally considered. Research should include also techno-economic and life cycle analyses.

Using mild conditions and non-toxic solvents is challenging. Chemocatalysis, producing now many petrochemical commodities, is used to apolar and unreactive feedstocks, conducting reactions in gas phase at high T and P; biomass implies instead oxygenated, reactive polar molecules with water ubiquitously present in feedstocks. Enzymes are in better position here, while chemo-catalysts are more robust against thermodegradation.

Producing low-volume/high-value bio-based products, in contrast to high-volume/low-value ones frequently relying on cheap non-precious metal catalysts, is a key issue also for commodity markets, as it may allow sustaining an integrated bio-refinery model. Here homogeneous catalysis, even if using costly precious metals (Ru, Ir, etc.) but with well-established synthetic methods, can come into play.

Intensification of processes to increase efficiency, lower the production costs and improve viability and energy and environmental efficiencies is also challenging. Implementing continuous processes in conventional flow reactors increases the productivity, but using micro- or structured reactors is a challenging step forward.

Another possibility is synthesizing bioproducts in electrolytic cells. O_2 and H_2 can be made in-situ from water using renewable electricity (photovoltaic or wind); using non-precious metal electrocatalysts in neutral pH and concentrated solutions to improve efficiency and developing cost-effective purification procedures are the challenges here.

Catalysis producing renewable building blocks from biomass
Bio-based industry might replicate oil-refineries, as the chemicals that our society needs are now made directly from oil. Bio-commodities produced via chemical catalysis (e.g. furfural, sorbitol, xylitol) are now in the market, from which other chemicals can be made; other compounds (levulinic acid, propylene glycol, etc.) are not yet cost-competitive (Ahorsu, 2018). Bioethanol or lactic and succinic acids, made via fermentation, are also in the market and could become platforms for other renewable chemicals; cheap glycerol from the biodiesel industry may also allow accessing multiple products at affordable prices. Developing efficient catalysts to achieve transforming all these platforms to valuable products is a vast and challenging field of investigation for the future.

Accessing cheap and widely distributed feedstocks
A widely-spread biomass feedstock is lignocellulose, a recalcitrant composite present in plant cell walls. It is built-up basically by lignin, a refractory aromatic polymer packing two polysaccharides: cellulose and hemicellulose (made up of different pentoses and hexoses). Cheap lignocellulose is widely available, but developing a cost-effective lignocellulose fractionation process to access this source of sugars and aromatics still remains a challenge. Bioethanol industry solved the problem, and has access to sugars breaking the lignin seal; but lignin, still recalcitrant, is used only for energy purposes.

Combining solvents and catalysts can fractionate lignocellulose, giving access to its sugar and aromatic content. Two chemocatalysis examples are the Triversa ProcessTM and the H_2-assisted Reductive Catalytic Fractionation; other possibilities are available (Schutyser, 2018). Lignocellulose degradation is catalysed by enzyme cocktails; oxidoreductases may depolymerise it. Protein engineering techniques can improve the activity and specificity of enzymes; advances are still needed to tailor these processes for the targeted products.

Other agro-food industry by-products can be also feedstocks, like chitin, a biopolymer present in crustaceans, mollusk shells and fungi cell walls; lactose-rich byproducts like cheese whey permeate; or marine seaweeds, also a good carbohydrate source. The challenge is to develop efficient and robust chemo- and bio-catalytic technologies converting these residues in added-value renewable chemicals.

Deploying the 2nd and 3rd generation biofuels

Lignocellulosic bioethanol and used cooking oil (UCO) biodiesel account for most 2nd generation biofuels consumed in Europe. Fuels from synthesis gas (or syngas; from now on, SG), a mixture of mostly CO and H_2 which can be derived also from biomass, are close to be cost-competitive (see Challenge 5 for details); also the interest in biofuels for air and marine transport (Fischer-Tropsch fuels, Hydrogenated Vegetable Oil kerosenes) is growing. The latter process needs noble metal catalysts to transform/crack the oil molecule; non-precious metal catalysts are needed here.

Concerning 3rd generation biofuels (obtained from microalgae), the real problem is the growing and harvesting of dry biomass at affordable cost; heterogeneous catalysts must also cope with interferences by phosphor- and sphyngo-lipids present in microalgae oil.

4. CATALYSIS FOR THE PRODUCTION OF CLEAN FUELS FROM RENEWABLE SOURCES

4.1. Catalytic production of SG from renewable sources

The new energy scenario requires replacing fossil carbon resources by carbon-neutral renewables. Options involving production and then conversion of SG to fuels and chemicals stand out as most attractive. Producing SG from non-food biomass, or from captured CO_2 (which can be a source of CO via the Reverse Water Gas Shift reaction, RWGS) and H_2 (made by water electrolysis) appears as an attractive option.

Impact in basic science panorama and potential applications. Key challenging points

SG from biomass gasification or pyrolysis usually contains impurities (N_2, CO_2, hydrocarbons, tars, etc.) and potential catalyst poisons (containing S, Cl, etc.) requiring costly cleaning pre-treatments. Adjusting the H_2/CO ratio in biomass-derived SG using e.g. downstream RWGS reactors, membrane separators or pressure swing adsorption may be necessary prior conversion to fuels or chemicals. Producing clean SG with the proper H_2/CO ratio requires optimizing process parameters and catalysts, adjusting them to all ranges of biomass feedstocks; using modular and scalable microreactors is a promising approach. For production of synthetic fuels, efficiently integrating the stack producing SG with the SG-to-fuels conversion reactor is another challenge to be addressed.

SG production from CO_2 and H_2O using C-neutral electricity is challenging (see sections C2 and D1 below). Cutting electrochemical cell fabrication costs, increasing cell efficiency and durability and developing new electrodes with better mass transport and overvoltage can allow a real, large-scale, one-stage SG production technology.

SG might also be produced by thermolysis of CO_2 and H_2O at high Ts using solar or nuclear reactor heat, but the O_2 produced needs to be removed from CO+H_2. Thermochemical cycles using oxides allow higher energetic efficiency, easier SG/O_2 separation and better process security. Redox pairs stable at high T (ferrites, CeO_2...) or showing phase transitions during reduction (e.g. Zn/ZnO) are promising. New materials should work efficiently at lower T, minimizing volatilisation and/or melting. Increasing the solar-to-fuel energy efficiency is a main challenge here. Photon-driven schemes can also convert CO_2 and H_2O into clean fuels; see section 5.2.

4.2. Catalysis converting CO_2 to useful products

Efficient routes converting CO_2 to fuels and chemicals are needed to reduce emissions of CO_2. (Kondratenko, 2013) A description follows of relevant catalytic routes for CO_2 transformation.

Impact in basic science panorama and potential applications

Conventional catalytic routes for CO_2 reduction

The mature Sabatier process hydrogenates CO_2 to CH_4 at mild Ts (150-500 °C) and pressures from 1 to 100 bar. One challenge here is improving catalyst resistance to coke and sulphur. New routes, still at early stages (TRL 3-4), use photothermal catalysts, e.g. Ni/g-C_3N_4 (operating at mild Ts) or $In_2O_{3-x}(OH)_y$.

Methanol production is interesting as it can be transformed to a variety of chemicals and fuels and has high energy density. The typical catalyst for methanol synthesis from SG, Cu/ZnO/Al_2O_3, works at 10-50 bar and mild T (200-280 °C); it can be modified to work with CO_2/H_2 blends by replacing Al_2O_3 with other oxides. Catalysts using reducible oxides are also good for CO_2 hydrogenation to methanol at high T (~400 °C). Other chemicals like formic acid (allowing H_2 storage) and dimethyl ether (DME) can also be made by CO_2 catalytic hydrogenation. This mature process still needs better resistance to coking and the water by-product.

Fischer-Tropsch synthesis (FTS) can be fed with CO_2 and H_2; combining its catalysts with acidic ones like ZSM-5 can lead to liquid fuels with narrow hydrocarbon distribution. Reducing directly CO_2 to aromatics and olefins (key building blocks in petrochemistry) is possible but challenging. Dry reforming of CH_4 with CO_2 (DRM), operating at Ts around 750 °C over Ni-based catalysts, can also produce SG. A chemical looping scheme for DRM, still under development, has resulted in better resistance to coking.

Catalytic processes for the conversion of CO_2 and H_2O mixtures

Electrocatalysts using renewable electricity can convert directly CO_2, but they still operate at high overpotentials, have low current densities and may deactivate easily; see sections 4.2 and 5.1 below. Solid state electrochemistry may convert CO_2 at high T to several products (CH_4, SG, larger molecules) with better kinetics and lower overpotential; electrodes based on complex perovskites show here good performance.

Photoreduction of CO_2 with water, named also artificial photosynthesis (AP), is a very challenging but appealing way for obtaining fuels. It is addressed, with or without help of electricity, in part 5.2 below; such technology remains still at lab scale (TRL 3-4). As for electrocatalysis selectivity, stability or high overpotentials remain still issues.

Processes incorporating CO_2 into chemicals and polymers
One niche for the industrial use of CO_2 is the synthesis of organic carbonates. This avoids using toxic phosgene to make dimethyl carbonate from methanol. The direct reaction is equilibrium-limited, but cyclic carbonates can be made reacting CO_2 with an epoxide using ammonium halide catalysts. Ethylene oxide can be converted to diethyl carbonate with MgO catalyst and by transesterification into a polymer, as in commercial synthesis of Bisphenol A-based polycarbonate. Making poly(ether carbonate) polyols from propylene oxide and CO_2 is also feasible using Zn based catalysts.

Also homogeneous catalysts can insert CO_2 in organics. Examples are N-formylation and N-methylation of amines; reductive formylations or methylations using hydrosilane reductants can be made with transition metal-based and metal-free catalysts. H_2 can be used as reductant, but the use of non-noble metal-based catalysts remains a challenge. Urea derivatives (e.g. carbamates) can be made from CO_2 also with organocatalysts.

Utilization of CO_2 as mild oxidant
Hydrocarbon dehydrogenation (DH) allows getting olefins and aromatics. This needs high Ts (600-700ºC), causing rapid catalyst deactivation by coking. Use of CO_2 as a milder oxidant for ODH (CO_2-ODH) avoids flammability and overoxidation and reduces coking, reducing also the reaction endothermicity. Two main catalyst types studied are those based on classical DH ones (Cr_2O_3 or Ga_2O_3) and on CeO_2 oxides.

Key challenging points
Developing a new generation of catalysts for CO_2 conversion
Most catalysts used in CO_2 hydrogenation are already efficient, but work to improve durability and selectivity and reduce costs is needed. Synergy with processes like production of renewable H_2, improving energy efficiency or bringing technologies to high TRL(8-9) by cooperating with international companies will also be needed. The impact of different CO_2+H_2 routes will depend on the availability of renewable H_2 and electricity.

Concerning solar fuels (obtained via AP), designing better photo-(electro)catalysts boosting energy conversion yields is key to bring technologies from current TRL 3-4 to TRL 6-7 so as to reach commercial level. Using CO_2 via direct solar activation of catalysts will continue to be a hot topic, but many of its basic aspects are still badly understood; real breakthroughs are needed to replace technologies using H_2. Other catalytic processes converting CO_2 can gain industrial relevance in niche applications (e.g. polycarbonates, making olefins). Finally, developing new multifunctional catalysts or smart process couplings can reduce for all technologies the number of steps for transforming CO_2 into fuels and chemicals.

4.3. Catalysts for obtaining clean hydrocarbon fuels and oxygenates from SG

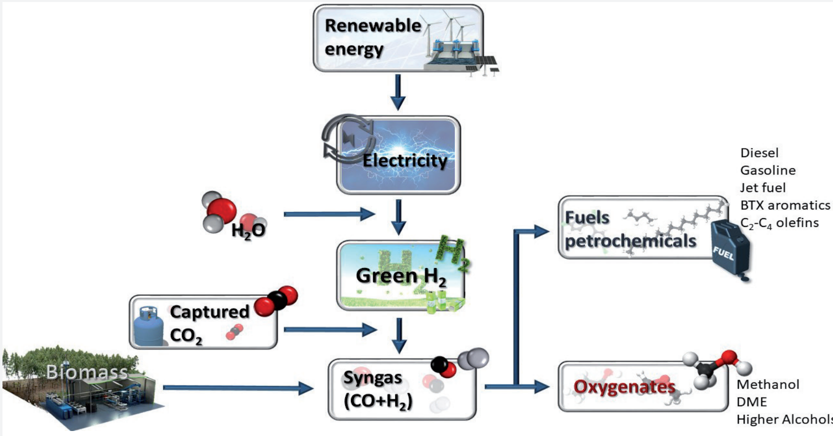
Catalytic SG conversion is one pillar in the chemical industry for producing clean fuels and value-added chemicals. SG is obtained now from fossil resources (>95%); its production from biomass and CO_2 (see previous sections) and the increasing use of renewable H_2 will give new chances for developing flexible and viable small scale processes with lower carbon footprint. Designing catalysts with better activity, selectivity and stability will be a key factor to improve the existing processes. Figure 5 below summarizes the renewables-to-SG-to-products main routes.

Impact in basic science panorama and potential applications. Key challenging points

Converting SG (from fossil sources) to liquid fuels via Fischer-Tropsch synthesis (FTS) is a mature technology (TRL 9); FTS processes using SG from renewable CO_2 have a lower degree of maturity (TRL 5-9); a deeper knowledge of active sites and reaction mechanisms, with advanced operando techniques and theoretical methods, is still needed here. Due to polymerization kinetics FTS products usually follow the so-called ASF distribution, limiting the attainable selectivity to a specific liquid fuel. FTS processes operate at conditions that generate mainly waxes; these can be subsequently upgraded in a downstream hydrocracker. The expensive hydrocracking step can be avoided with catalysts including a FTS catalyst and a zeolite to transform, via acid-catalyzed cracking and isomerization, FT-derived waxes. This approach has not yet achieved commercialization due to fast zeolite deactivation; further developments in this area are anticipated.

SG conversion can also make light olefins and aromatics, key building blocks for the petrochemical industry. Lower olefins can be made from SG in a single reactor via a high-T FT-to-olefins (FTO) process using iron catalysts.

FIGURE 5–Possible routes for renewables-to-SG-to-products processes. Source: freely elaborated and adapted by M.A. Centeno with a student of his, starting from Z. Jiang, T. Xiao, V. L. Kuznetsov, P. P. Edwards: Phil. Trans. R. Soc. A (2010) 368, 3343; and G. Leonzio: Waste and Biomass Valorization, doi: 10.1007/s12649-019-00914-4. With due permissions.



Improving the selectivity to C_2-C_4 olefins while lowering CO_2 formation, as well as enhancing the lifetime and integrity of Fe-based catalysts in these harsh conditions are major challenges in this process. Another route exists via oxygenated intermediates. It needs bifunctional catalysts coupling a methanol synthesis (MS) catalyst and a methanol-to-olefins (MTO) zeolite catalyst. Non-Cu-based catalysts (e.g. ZnO-ZrO_2) are better than Cu-based systems, being active at higher Ts as is required for MTO; deactivation of MTO catalysts is however a key issue. Converting SG to aromatics is feasible using dual-function catalysts, the choice of catalysts depending on the pathway intermediates: oxygenates or light olefins. Catalysts for the olefins route mix a Fe-based FTO catalyst with a Ga_2O_3- or ZnO-modified zeolite ZSM-5 catalyzing the aromatization of the formed olefins. For the oxygenates route bifunctional systems mixing a methanol/DME catalyst like ZnO-ZrO_2 and ZSM-5 zeolite are promising. Further studies to improve the aromatics productivity and the selectivity to the demanded para-xylene isomer will be needed.

The SG to methanol route is a mature technology using Cu/ZnO/Al_2O_3 catalysts. However, devising new catalysts with better activity at lower T and pressure, selectivity, stability and resistance to poisons, and gaining understanding on the reaction mechanism, nature of active sites and promoter effects are still scientific and technical challenges. DME is, besides methanol, a key intermediate in chemical industry, usually obtained by a two-stage process: i) methanol synthesis from SG and ii) methanol dehydration. The growing interest in using DME as a clean fuel replacing oil-derived LPG and diesel has promoted developing a one-step process (STD: SG-to-DME), a relatively mature technology. This process is more competitive and thermodynamically favorable, enabling higher per-pass CO conversions. STD catalysts are bifunctional, comprising a Cu-based methanol synthesis catalyst and alumina or, preferably, zeolites. Fine tuning of zeolite acidity and porosity to suppress coking and a good integration with the Cu catalyst are needed to improve DME selectivity and catalyst lifetime.

Higher alcohols are valuable compounds with uses in the chemical, pharmaceutical and energy industry. Their direct synthesis from SG can give a more environmentally friendly, versatile and economic alternative to their current production by fermentation of sugar or hydration of oil-derived olefins. Catalysts developed for this process can be classified in four categories: i) Rh-based, ii) Mo-based, iii) modified FTS, and iv) modified methanol synthesis catalysts (Luk, 2017). Mo-based systems (mostly alkali-promoted MoS2) appear most promising in cost/performance terms; further improvements in catalyst design are expected to shift alcohol distribution from methanol to the desired higher alcohols. Future studies here should focus on a better understanding of the nature of active sites and mechanisms, to guide the design of better catalysts. Better reactor and separation technologies will also be needed for a real industrial implementation.

5. ELECTRO/PHOTO/CATALYSIS FOR ENERGY CONVERSION

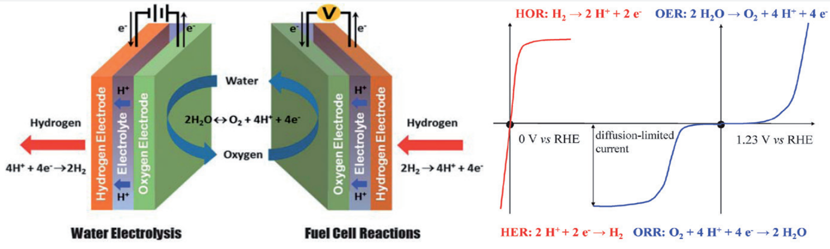
5.1. Catalysts for fuel cells and electrolysers

The performance and cost of fuel cells (FC) and electrolytic cells (EC) depend on the performance and cost of their electrocatalysts. These devices can be classified in three classes: low T (<200ºC), including proton membrane exchange (PEM) and alkaline cells; intermediate T (400-800 ºC), mostly using proton conducting or solid oxide electrolytes; and high T (>800º) solid oxide (SO) cells. See Figure 6 below for PEMFC and EC schemes. Reviews are available for PEM and SOFC (Ioroi, 2019), (Sreedhar, 2019)

Impact in basic science panorama and potential applications

Most FCs use pure H_2 or H_2-rich gases as fuel (including CO, although CO is a poison for Pt catalysts used in PEMFCs); some devices use other fuels,

FIGURE 6–Scheme of PEMFC and PEMEC, and polarization curves of the main electrode reactions. Sources: S. Park, Y. Shao, J. Liu, Y. Wang, Energy Environ. Sci. (2012) 5, 9331; Y. Jiao, Y. Zheng, M. Jaroniec, S.Z. Qiao, Chem. Soc. Rev. (2015) 44, 2060. With due permissions.



bioethanol being the most interesting one for low T FCs. Most EC developments produce H_2 from renewable electricity (and this H_2 can be catalytically converted to liquid carriers, and then back, for its easier transportation), and some prototypes produce SG by co-electrolysis of water and CO_2; other catalysts like Cu, Zn or Sn can give other products of CO_2 reduction, from formic acid to CH_4 or C_2+ hydrocarbons. For cases where weight and size are limited, unitized regenerative fuel cells (URFC) combine fuel cells and electrolysis in one device. For portable applications micro-FCs are being developed, some of them without membrane for use in disposable devices.

Carbon-supported Pt is a standard catalyst for both electrodes of PEMFC; PEMEC anodes require Ir supported on non-carbon materials (like Ti-based structures) due to corrosion by O_2. Alkaline EC, the most mature electrolysis technology, uses Ni-based electro-catalysts. Alkaline membrane technology for FC and EC is still in progress, due to the low conductivity and stability of such membranes, but the higher kinetics in the oxygen electrode holds promise for application of lower cost catalysts. High T SOFC and SOEC electrodes use similar electrocatalysts, e.g. a cermet of Ni metal and the electrolyte (yttrium stabilized zirconia, YSZ) for the H_2 electrode; a La-Sr-Mn perovskite oxide for the O_2 electrode. URFCs are mainly PEM-type, combining FC and EC materials (Pt-Ir supported in Ti compounds) for the O_2 electrode. Finally, direct-ethanol fuel cells (of PEM-type) require a bimetallic catalyst (Pt-Ru or Pt-Sn) in the anode.

EC and FC electrodes have several common features: high electronic conductivity; high ionic conductivity, for an effective connection with the electrolyte; and tailored porosity, for the mobility of reactants and products to and from the catalytic active site. The electrode conformation should include the active catalysts with these characteristics.

The electrochemical synthesis of NH_3 from N_2 and H_2O at ambient T (Hou, 2020) deserves now much attention. The technology is still starting, but has high interest if it can compete with the Haber-Bosch process needing high Ts and pressures.

Key challenging points

Alkaline EC is well established; although improvements are possible in the electrodes conformation. PEMEC have much higher efficiency and allow better integration with renewable energies due to a greater operation range. The high cost and scarcity of catalysts and the electrode durability are the main barriers for the competitiveness of PEMFC and EC. PEM is the most advanced FC technology, but only motor vehicle companies provide commercial products reliable enough. Using non-precious metal catalysts, especially for alkaline membrane FC and EC, and increasing the intrinsic activity using multicomponent nanostructured catalysts are two of the main objectives.

High T SOFC and SOEC electrodes have problems of compatibility with the electrolyte, due to different thermal expansion coefficients. Besides, high T migration of La and Sr from the SOFC cathode to the electrolyte interface degrades the cell. The low ionic conductivity of the catalytic layer is also a handicap. Also, manufacturing of high T electrodes increases the final cost of the devices. Finally, there is much interest in lowering the T operation range of SOFC, to allow using cheaper construction materials and increasing the stability with time at lower Ts.

The practical use of the rest of the FC and EC are further away. Direct ethanol FC catalysts have very low activity and selectivity to total electroxidation, so that these FC are unpractical as energy equipment; URFC need specific bifunctional catalysts (anodic-cathodic) for the O_2 electrode; and there is scarce information about the appropriate electrocatalysts to be used in the intermediate T fuel cells.

Scale-up of electrode manufacturing is of key importance for final commercialization. Current procedures rely on wet chemical, liquid printing, ceramic, sol-gel or related chemical methods, but some of them are costly for large scale production. Others based on physical surface treatments (e.g. magnetron sputtering) might be also considered.

Finally, although there is a great knowledge of the electrochemical behaviour of model surfaces, the whole understanding of the electrochemical processes in real catalysts working in real cells is far away to be reached.

5.2. Photon-induced water splitting and CO_2 reduction

Photocatalysis is used for environment protection, selective synthesis or energy-related aims; in the latter case, it allows fixing photon energy in chemical form. Such "artificial photosynthesis" (AP) can follow two ways: H_2 production (by H_2O splitting or photo-reforming) or CO_2 reduction, both providing "solar" fuels and chemicals.

Impact in basic science panorama and potential applications.

A *purely photocatalytic process* fixing energy has high potential due to scalability and high efficiency, but does not compete yet with other routes. Also separating oxidation and reduction products can be difficult, except in photo-reforming of organics where value-added chemicals besides H_2 can result. This process works at milder T than thermal reforming, saving thus energy especially if using sunlight. A special case is that of homogeneous photocatalysis using elaborate metal complexes (which may try to mimic enzymes) combined with a molecular photon absorber, as e.g. for H_2 production or synthesis of NH_3 using protons plus electrons provided by the absorber. Photocatalysis can be however combined advantageously with other technologies (e.g. thermo-, electro-) into photothermal and photoelectrochemical catalysis.

Photothermal CO_2 reduction is a recent double route using both light and heat activation. Heat can be obtained directly from an external source (e.g. a solar concentrator) or by light absorption (e.g. by surface plasmon resonance). Coupling to a semiconductor with ability for photo e^-/h^+ pair generation and charge transfer gives good activities, e.g. in methane production via Sabatier reaction ($CO_2 + 4\,H_2 \rightarrow CH_4 + 2\,H_2O$) on oxide-supported metal catalysts at mild Ts under UV-visible light.

Photoelectrochemistry (PEC) is used for water splitting or CO_2 reduction. One electrode containing a light absorber (or two in tandem systems) is iluminated driving chemical changes. PEC electrodes reducing H^+ to H_2 or CO_2 to a fuel require conduction band potentials more negative than the relevant redox pair; valence bands of those doing oxidation must be more positive than the O_2 couple. Co-catalysts are needed, like in electrolysis, to lower reaction barriers. MoS_x or metal alloys work for H_2 evolution; Zn, Ag, Cu or Sn (depending on the sought products) for CO_2 reduction; Ni, Co or Fe oxides for O_2 evolution. Enzymes (formate dehydrogenases, laccases, hydrogenases...) can also serve as co-catalysts. All this may result in complex multilayered electrodes.

Key challenging points

For these technologies light absorbers with somewhat lower bandgaps, more efficient co-catalysts and better carrier separation efficiency are required. For all photodriven processes better band edge (or redox levels of complexes) positions versus redox pairs are needed, as well as smart, more compact photoelectrode designs in PEC. In photothermal CO_2 reduction it is also necessary to lower the T window.

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TABLE 1—List of challenges to be addressed for the Challenge 7

		NEAR TERM (<5YEARS)	MID TERM (5-10 YEARS)	LONG TERM (10-20 YEARS)
CATALYSIS FOR A SUSTAINABLE INDUSTRIAL PRODUCTION	**Catalysis for industrial production with lower energy demand and higher atom efficiency**	• Obtaining better selectivity to the desired products using improved homogeneous and heterogeneous catalysts • Allow operation at milder P and T conditions	• Improving enzymes through directed evolution; better stabilization of them on specific solid carriers, allowing cascade processes. • Process intensification, integrating chemical and physical steps to achieve better energy efficiency	• Improving largely atom efficiency, so that separation and purification steps can be reduced
	Air depollution in energy-intensive industries	• Replacing noble metals by less costly transition metal oxides in catalysts burning VOCs. • Development of new catalysts to avoid N_2O emissions during fertilizers production. • NOx: Development of new low-temperature SCR catalysts for use in tail gas systems.	• Activation of catalytic materials by photons or microwaves to avoid heating all the gas mass	
		CROSSCUTING ACTIVITIES		
		• Design and manufacture of improved catalysts through simulation and controlled synthesis of nanoparticles by new methods. • Use of real-time spectroscopy and chemometric analyses and operando methods at lab scale and pilot plants for developing catalysts and process control in their industrial manufacture and use.	• New techniques for structuring solids by means of 3D additive manufacturing.	

		NEAR TERM (<5YEARS)	MID TERM (5-10 YEARS)	LONG TERM (10-20 YEARS)
CATALYSIS FOR A SUSTAINABLE INDUSTRIAL PRODUCTION	**Processes directly driven by electricity and electromagnetism**	• Improving the knowledge about the interaction between MW/plasma/ magnetic fields and reactants/catalysts. • Improving basic parameters of the reaction such as energy efficiency and selectivity.	• New reactor designs able to treat large volumes of reactants. Improving the control of applicators and process command. • Developing new catalysts specific for electricity-driven catalysis. • MW-specific: Implementation in complex processes and development of automatic control	• Useful engineering solutions for an efficient connection to the electricity grid. • MW-specific: Study of new reactions not achievable today; use of phase mixtures (gas, liquid, solid, plasma); microreactors operated by batteries.
CATALYSIS FOR THE USE OF BIOMASS	**Production of biofuels and chemicals from biomass**	• Developing technologies to produce bio-based products either form previous building blocks or directly from biomass (up to TRL 4). • Techno-economic and LCA analysis of the above-mentioned technologies to assess on their economic and environmental viability and to identify the bottle-necks for further improvements	• Improvement of the most promising technologies to tackle down the bottle-necks identified by the techno-economic and LCA analyses (up to TRL 6).	• Scaling-up and intensification of the technologies up to TRL 7-8.
	Renewable building blocks from biomass	• Developing environmentally friendly technologies to produce bio-based building-blocks (up to TRL 4). • Techno-economic and LCA analysis of the above-mentioned technologies to assess on their economic and environmental viability and to identify the bottle-necks for further improvements.	• Improvement of the most promising technologies to tackle down the bottle-necks identified by the techno-economic and LCA analyses (up to TRL 6).	• Scaling-up and intensification of the technologies up to TRL 7-8.

		NEAR TERM (<5YEARS)	MID TERM (5-10 YEARS)	LONG TERM (10-20 YEARS)
CATALYSIS FOR THE USE OF BIOMASS	**Accessing cheap feedstocks**	• Developing at least two environmentally friendly catalytic (chemo• or enzymatic) technologies efficiently fractionating cheap lignocellulose feedstocks into carbohydrate and lignin (up to TRL 4). • Developing at least two environmentally friendly technologies to process cheap non-lignocellulosic feedstocks (chitin, cheese whey permeate or marine seaweeds) into valuable chemicals (up to TRL 4). • Techno-economic and LCA analysis of the technologies to identify the two most viable technologies and the environmental and economic the bottle-necks for further improvements	• Improvement of the two most promising technologies to tackle down with the bottle-necks identified by the techno-economic and LCA analyses (up to TRL 6).	• Scaling-up and intensification of the technologies up to TRL 7-8.

		NEAR TERM (<5YEARS)	MID TERM (5-10 YEARS)	LONG TERM (10-20 YEARS)
CATALYSIS FOR THE USE OF BIOMASS	**2nd and 3rd generation biofuels**	• Developing environmental-friendly catalytic or enzymatic technologies to produce biodiesel from UCO and HVO kerosene from (preferably) microalgae (up to TRL 4). Catalysts for the latter process must be based .on non-precious metals. • Techno-economic and LCA analysis of the above-mentioned technologies to assess on their economic and environmental viability and to identify the bottle-necks for further improvements.	• Improvement of the most promising technologies to tackle down the bottle-necks identified by the techno-economic and LCA analyses (up to TRL 6).	• Scaling-up and intensification of the technologies up to TRL 7-8.
CATALYSIS FOR THE PRODUCTION OF CLEAN FUELS FROM RENEWABLE SOURCES	**Production of syngas from renewable sources**	• Development of optimized catalysts, reactors and processes for SG production from residual biomass and/or CO_2 + H_2O.	• Achieving an efficient SG production from CO_2 and H_2O using C-neutral electricity.	• Reaching the threshold yield for commercial exploitation of SG production from photo(electro) catalytic processes and other promising advanced technologies from CO_2 + H_2O. • On-demand production of SG with the appropriate characteristics for its final use, from localized and specific residual biomass. • Emergence of new catalytic processes for economical SG production with zero carbon footprint.

		NEAR TERM (<5YEARS)	MID TERM (5-10 YEARS)	LONG TERM (10-20 YEARS)
CATALYSIS FOR THE PRODUCTION OF CLEAN FUELS FROM RENEWABLE SOURCES	**Converting CO_2 to useful products**	• Broad deployment of optimized catalytic processes for Power-To-Gas and Power-To-Liquids technologies. • Design of more efficient catalyst for CO_2 utilization in chemical production.	• Improvement of catalysts and scaling up of transformation routes, particularly those for implying direct solar CO_2 activation. • Development of hybrid CO_2 conversion routes by synergic coupling of processes.	• Reaching the threshold yield for commercial exploitation of photo(electro) catalytic processes and other technologies for CO_2 + H_2O conversion. • Emergence of novel catalytic schemes for CO_2 conversion.
	Obtaining clean fuels and oxygenates from syngas	• Gaining in-depth understanding of catalyst structure-performance relationships. • Developing efficient multifunctional catalysts for direct (one-step) SG conversion with high selectivity to target products (process intensification).	• Demonstration plants for direct conversion of SG to liquid fuels and chemicals. • Deployment of new SG conversion technologies using renewables.	• Scaling-up of cost-effective sustainable SG conversion technologies based on renewables with low or neutral carbon footprint.
ELECTRO/PHOTO/ CATALYSIS FOR ENERGY CONVERSION	**Catalysts for fuel cells and electrolysers**	• Optimum electrode conformation for alkaline electrolysers. • Electrodes for PEMFC with low Pt content (under 0.15 g/kW). • Durable electrodes for solid oxide fuel cells and electrolysers (higher than 40.000 h).	• Active and durable electrodes, based in non-precious metal catalysts, for low temperature fuel cells and electrolysers. • Low cost methods for manufacturing components for high temperature fuel cells and electrolysers (e.g., based on physical surface treatments). • Deciding whether there is promise in schemes for production of NH_3 via electrolysis	• Development of practical electrocatalysts for direct ethanol fuel cells.working in real cells. • Development of low cost bifunctional electrocatalysts for URFC. • Whole understanding of the electrochemical processes in real catalysts.

		NEAR TERM (<5YEARS)	MID TERM (5-10 YEARS)	LONG TERM (10-20 YEARS)
ELECTRO/PHOTO/ CATALYSIS FOR ENERGY CONVERSION	**Photon-induced water splitting and CO_2 reduction**	• Developing light absorbers with lower bandgaps and providing better carrier separation efficiency; and more efficient co-catalysts.	• Developing smart, more compact photoelectrode designs in photoelectrochemical reactors. • Reducing the working temperature for the photothermal CO_2 reduction.	• Developing photo(electro) catalysts with high efficiency for water splitting, using materials with an optimized life cycle. • Suppressing the use of sacrificial compounds for O_2 evolution in water splitting photoreactors.

ONE SLIDE SUMMARY FOR EXPERTS

Challenge

This challenge deals with catalysis (heterogeneous, homogeneous and enzymatic) as applied to energy purposes: clean fuel synthesis from renewables, carbon dioxide transformation to obtain fuels and chemicals, use of electricity in conventional (e.g. electrolysis) and less common (e.g. microwaves, plasmas) ways, use of biomass, solar energy driven processes, atom- and energy-conserving economy... The specific challenges are very different, as are these applications, relating mainly to the need of developing catalysts behaving more efficiently, with high selectivity, working in milder conditions, being more durable and using (if possible) earth-abondant elements.

Approach

One first general approach involves designing advanced catalyst synthesis methods (microemulsions, fibers, single-atom species, control of interaction with carriers...), characterizing catalysts with a high variety of structural and spectroscopic techniques (including *operando*), multiscale modelling of reactions (maybe with machine learning and AI), design of advanced reactor types (with multiple narrow channels, for photocatalysis, gas diffusion electrodes for fuel cells, etc.). Then each energy-oriented application has specific needs: biomass use requires cheap but selective processes; electrolyzers and fuel cells require low overpotentials; plasmas must be able to use large gas amounts; clean fuel synthesis needs different selectivity for different fuels...

Social and economic impact

- Catalysis may help to decrease pollution, both by greenhouse gases (CO_2, CH_4, N_2O) and toxic substances (NO_x, CO, dioxins, herbicides, ...), improving people's well-being
- Catalysts may lead, first of all, to processes which are cheaper and consume less energy and material resources. This will already have large economic consequences
- The changes coming to chemical industry will lead to suppression and creation of jobs
- The social awareness of the importance of technology must increase; this is especially true for the climate change issue, which will lead to changes in energy, migrations, etc. Education plays a key role here
- Electricity generation (by windmills, PV fields, etc.) is already changing the landscape, as has happened already with its hydraulic generation.

José Carlos Conesa (Challenge Coordinator)

This should not be overlooked. Catalysts may also change gradually in composition; new mines may have then to be established while others may need being cancelled, impacting both landscape and jobs

Involved teams

Many groups in CSIC work on catalysis of different types. The main ones are located at ITQ and ICP, this latter institute being particularly active in enzymatic catalysis (besides the heterogeneous one); other important groups working significantly on heterogeneous catalysis and related systems exist in ICB, ICMSE, INCAR, IRNASE, ICN2, ICMM and ICMAB, while homogeneous catalysis is pursued mainly in ISQCH and IIQ. There are also other research centres working actively in catalysis; not only in universities, but also in other institutions like ICIQ and IREC in Catalonia, the IMDEAs in Madrid Community or the different technology centres in the Basque Country.

ONE SLIDE SUMMARY FOR THE GENERAL PUBLIC

Challenge

Catalysis was defined in the XIX century as the way to change the course of a chemical reaction by adding a substance that is not consumed in the process. This challenge deals with catalysis of different types as applied to energy purposes: clean fuel synthesis, fuel cells, use of biomass, carbon dioxide transformations, sunlight-driven processes to fight climate change… Its importance is glimpsed from phrases in a recent report by the European Cluster of Catalysis: "Of the 50 largest volume chemicals now produced, 30 are produced via catalytic routes… and account for more than 20 billion tons of CO_2 emitted yearly to the atmosphere… Technical improvements in catalyst processes could reduce energy intensity for these products by 20% to 40% by 2050."

Approach

The many possible uses of catalysis imply also many approaches to solve the different challenges. Some are common to all catalysis types: designing better catalyst synthesis methods, studying catalysts with structural and spectroscopic techniques, modelling catalytic reactions, performing studies of the reaction rates, designing new reactor types for catalysis… Then each energy-oriented application has specific needs: fuel cells need more durable catalysts and low (or none) amounts of precious metals, clean fuels synthesis requires directing the result to each fuel desired, biomass processes normally need a sequence of chemical reactions to end with the specific product sought, photocatalytic processes need high solar efficiencies; and so on.

Social and economic impact

- Catalysis may help to decrease pollution, both by greenhouse gases (CO_2, CH_4, N_2O) and toxic substances (NO_x, CO, dioxins, herbicides, ...).
- Catalysts may allow processes which are cheaper and consume less energy and material resources.
- The changes produced to the chemical industry will lead to suppression and creation of jobs; it is expected that the latter will be in higher numbers and more specialized.
- The social awareness of the importance of a better technology must increase; education plays here a key role. The climate change issue, leading to changes in energy use, society transport models, migrations, etc. is particularly relevant here.
- Electricity production (by windmills, solar panels) is changing landscape, as happened already with hydraulics. The debate on concentrated vs. distributed energy generation, and changes in mining needed for producing new catalysts, will have also impact here.

Involved teams

Many groups in CSIC work on catalysis of different types. The main ones are located at ITQ and ICP, this latter institute being particularly active in enzymatic catalysis (besides the heterogeneous one); other important groups working significantly on heterogeneous catalysis and related systems exist in ICB, ICMSE, INCAR, IRNASE, ICN2, ICMM and ICMAB, while homogeneous catalysis is pursued mainly in ISQCH and IIQ. There are also other research centres working actively in catalysis; not only in universities, but also in other institutions like ICIQ and IREC in Catalonia, the IMDEAs in Madrid Community or the different technology centres in the Basque Country.

CHALLENGE 8

HYDROGEN TECHNOLOGIES

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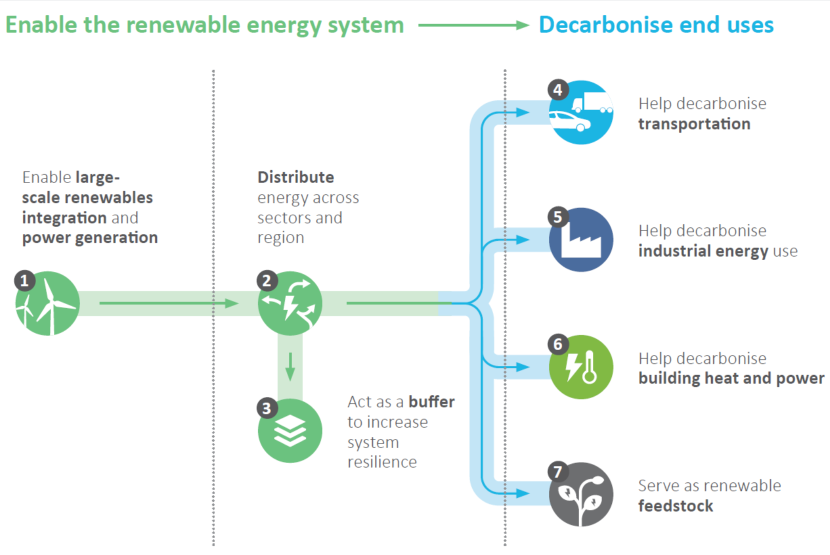
1. INTRODUCTION

Hydrogen, as an energy carrier, is a clean and storable solution that could decarbonize several economic sectors presently based on fossil fuels. Hydrogen is a very promising option to decarbonize transport including, cars, buses, trucks, trains, ships etc, where batteries present important disadvantages: higher initial and maintenance cost, lower energy density, and slow recharging performance. In addition, the transport sector produces around one-third of all CO_2 emissions, thus, decarbonization of this sector is a key element in achieving limitations in global warming.

Hydrogen can also be an important input for specific industries where energy-intensive processes are present. In steelworks, hydrogen can substitute coal as reductant. For ammonia production, hydrotreating in refineries and methanol production, hydrogen is used as feedstock. Hydrogen and CO_2 can also be used as feedstock for so-called electrofuels and can play an important role in the transition to renewables, providing mechanisms to seasonally store, transport and distribute energy throughout all sectors and continents, Figure 1.

Together with fuel-cell technologies, hydrogen offers an excellent opportunity for local industry to take advantage of nearby available renewable energy, to improve its technological development during the energy transition and to increase the economic value for regions. Although hydrogen technologies represent a promising alternative for decarbonization of the energy system and

FIGURE 1–Hydrogen can balance energy production and use in location and time, and decarbonize end uses (Hydrogen Council 2017).



stabilization of renewable energies, important obstacles need to be overcome for extensive deployment of hydrogen and fuel-cell technologies. These obstacles are mostly related to current costs of fuel cells, the development of efficient low-cost process to produce hydrogen with a low-carbon footprint, and the development of a wide and safe network for hydrogen transport and distribution.

Much of the hydrogen and fuel-cell technology is not yet commercially available or is still in the early stages of commercialization. In addition, it has to compete with alternative technologies with a relatively lower cost, which also present a low-carbon foot-print. Thus, further attention will be needed before their high potential can be totally realized. Governments can help accelerate the development and deployment of these technologies by ensuring the funding of fundamental and applied research, and demonstration projects for hydrogen generation, storage, distribution and uses, as well as promoting new policies to design, create and facilitate a hydrogen market, infrastructure and economy. The close collaboration among many stakeholders (i.e. oil and gas industry, utilities and power grid providers, car manufacturers, Technological centers, Universities, and local, regional and national authorities) will also be decisive to successful overcome the aforementioned barriers.

The present study in no way considers hydrogen as the only solution to achieve the energy transition, but rather as a key element of the portfolio of low-carbon technologies that could help to decarbonise the current energy system while enabling significant perspectives of growth for the economy. It also expects to identify the most promising short-, medium- and long-term opportunities, and provide orientation to encourage and promote CSIC research lines dedicated to hydrogen technologies.

2. HYDROGEN PRODUCTION

Primary energy sources useful for hydrogen production comprise renewable ones, such as solar, wind and biomass, and also fossil fuels, such as natural gas and coal.

2.1. Hydrogen from Fossil Fuels

Nowadays, most hydrogen is produced from fossil fuels. Specifically, natural gas accounts for around 75% of the annual global dedicated hydrogen production (around 70 million tonnes). Coal accounts for an estimated 23% of the global dedicated hydrogen production and uses 107 Mt of coal (2% of global coal use) (IAE Report for the G20 2019). The dependence on natural gas and coal means that hydrogen production today generates significant CO_2 emissions: 10 tCO_2/tH_2 from natural gas, 12-19 tCO_2/tH_2 from coal (IAE Report for the G20 2019).

Hydrogen can be produced from fossil fuels by steam reforming (SMR), partial oxidation, and autothermal reforming (ATR). Carbon Capture and Storage (CCS) can be applied both to SMR and ATR. Using CCS with SMR plants can lead to a reduction in CO_2 emissions of up to 90%. Several SMR-CCS plants are already operational, producing around 0.5 MtH_2/year in total (IAE Report for the G20 2019).

Hydrogen can be also produced from coal gasification, which, as in ATR plants, allows for a relatively easy capture of CO_2. However, coal gasification plants emit about four times more CO_2 per kg of hydrogen produced than ATR plants, increasing the amount of carbon that must be transported and stored (IAE Report for the G20 2019).

Impact in basic science panorama and potential applications

Natural gas steam reforming with CCS is an attractive and needed option for hydrogen generation, if the CO_2 price is above 45.9 €/tCO_2 (IAE Report for the G20 2019). Nowadays, hydrogen is produced by SMR at a cost of 2.10 €/kg if the carbon penalty is included. However, this price will increase up to 2.6 €/kg with a carbon penalty of 80 €/tCO_2 in 2025 (Fuel Cell and Hydrogen Joint Undertaking Report 2017). Hydrogen can be produced by ATR of natural gas with CCS at a price of 1.5 €/kg (Kayfeci, Keçebaş and Bayat 2019), while hydrogen produced by coal gasification is in the range 1.8-2.7 €/kg (Olateju & Kumar 2013).

Key challenging points

1. Produce hydrogen at target costs and with near-zero greenhouse-gas emissions.
2. Develop carbon capture, CO_2 storage, and CO_2 utilization technologies that ensure minimal carbon dioxide is released in the hydrogen-production process.
3. Improve the robustness and lifetime of ATR catalysts.

8.2.2. Hydrogen from biomass

Thermochemical and biochemical processes are the main routes to produce hydrogen from biomass. Gasification is a well-established technology involving heat, steam, and oxygen to convert biomass to hydrogen and other gases (CO, CO_2 and CH_4), without combustion (US Department of Energy 2020). In biochemical routes, microorganisms work on organic material to produce hydrogen, biogas or a combination of acids, alcohols and gases. Both biogas from biochemical routes and hydrogen produced from biomass gasification have a high content of CO_2 (10-25%) (US Department of Energy 2020), besides CH_4. Thus, the use of dry reforming of methane (reaction of CH_4 and CO_2 to produce syngas) is a very promising way to produce hydrogen and avoid CO_2 emissions. Reforming biomass-derived liquids (ethanol, glycerin, etc) is another interesting option to produce renewable hydrogen (US Department of Energy 2020).

Anaerobic digestion (AD) provides possibilities to produce renewable energy from organic wastes in decentralized sites, yielding a methane-rich biogas from manure (human and animal) and crop residues (US Department of Energy 2020). Apart from supplying renewable energy, AD plants have other positive effects including the strengthening of closed-loop recycling management systems, reducing emissions and producing a valuable organic fertilizer.

Impact in basic science panorama and potential applications

Since growing biomass removes CO_2 from the atmosphere, the net carbon emissions, when hydrogen is produced from biomass will be very low, especially if coupled with CO_2 capture. Although there are a number of biomass gasification demonstration plants in the world, the technology is not yet fully developed and the produced gas would need to be further processed to extract hydrogen. In addition, the potential for large-scale biomass-based hydrogen production is limited by the availability of cheap biomass.

Key challenging points

1. Reducing costs associated with capital equipment and biomass feedstocks. To increase the net efficiency, and to reduce the energy cost, hybrid technological approaches based on combined solar heat and gasification.
2. Reducing the cost and complexity of production of clean hydrogen and hydrogen-rich gases from biomass gasification.
3. For biomass-derived liquids, research is needed to identify better catalytic materials to improve yields, selectivity, robustness and lifetime.
4. There is also a challenge to make fermentation systems with higher hydrogen production rates and increase the yield of hydrogen.

2.3. Hydrogen production by water splitting

Hydrogen from water splitting is possible: (i) using renewable electricity (electrolysis); (ii) using solar thermal energy; and (iii) by direct water splitting using sunlight; or a combination of these methods.

Two main technologies for electrolysis cells (EC) are used: low temperature (<200ºC), including proton membrane exchange (PEMEC) and alkaline cells, and high temperature (>700ºC) solid oxide cells (SOEC) (European Energy Research Alliance 2019; Carmo, Mergel and Stolten 2013; Zeng & Zhang 2010; Laguna-Becerro 2012). For applications where weight and size are limited, unitized regenerative fuel cells (URFC) combine fuel cells and electrolysis in one device. The membrane-electrode assembly (MEA) is the heart of these devices. For PEMEC, Nafion® is the state-of-the-art electrolyte membrane. The electrodes are made of carbon-supported platinum (cathode) or iridium (anode) (Carmo, Mergel and Stolten 2013). Bipolar plates connect the different cells of a stack and allow the output of products. Alkaline EC is a more mature technology, using nickel electrodes and a KOH solution as electrolyte. If an appropriate membrane is developed, alkaline membrane EC, with a configuration similar to PEMEC, could produce lower cost devices (European Energy Research Alliance 2019; Zeng & Zhang 2010). MEAs for SOEC are ceramic: an electrolyte of yttrium stabilized zirconia (YSZ), a cermet of Ni-YSZ (cathode) and a La-Sr-Mn perovskite oxide (anode) (Laguna-Becerro 2012). Materials suitable for high temperature seals and electrical connectors are of paramount importance.

For the direct thermal splitting of water, a temperature higher than 4000ºC is need. Lower temperature (<1000ºC) is possible if thermochemical cycles are used, with a series of chemical reactions in a closed cycle. Several cycles have been proposed, requiring a water reduction to hydrogen step, and another reduction step of some of the involved compounds where oxygen is produced (European Energy Research Alliance 2019; Safari & Dicer 2020).

Water splitting by direct solar light requires a photocatalyst, with an energy gap (valence-conduction bands) appropriate for absorbing sunlight and transferring electrons to the protons of water (European Energy Research Alliance 2019; Hisatomi, Kubota, and Domen 2014). This process can be accomplished using electrical energy (photoelectrical splitting), which produces a bias potential in the catalysts that favour the photocatalytic yield.

Impact in basic science panorama and potential applications

Water splitting is the most appropriate manner to produce hydrogen in the future massive deployment of renewable energies. Electrolysis combined with photovoltaic, waves, hydro, or wind electricity will open the door to power-to-gas technologies, allowing the seasonal storage of renewable energy, regulation of the electrical network, and distribution of energy to the transport sector.

The bottleneck is the production price of renewable hydrogen, which is currently higher than 5 €/kg (IAE Report for the G20 2019; Fuel Cell and Hydrogen Joint Undertaking Report 2017; Kayfeci, Keçebaş and Bayat 2019) far away from 2.1 €/kg for SRM (carbon penalty included). However, the development of new materials for electrolysers and their industrial manufacture, seem to indicate that this price will be reduced to 2.0-2.2 €/kg for hydrogen produced from photovoltaic energy in Spain (IAE Report for the G20 2019).

Key challenging points

1. Development of alkaline membranes and a proton exchange membrane alternative to commercial Nafion®, of lower cost and higher durability. Production of bipolar plates/diffusion layers of low cost and high corrosion resistance. Improving chemical stability and durability of the components of solid oxide electrolysers.
2. Materials with a high capacity of recycling, with the lowest amount of single steps and using environment-friendly compounds for thermochemical cycles. Photo(electro)catalysts of high efficiency and optimum life cycle, without sacrificial compounds for the evolution of oxygen.

3. STORAGE AND DISTRIBUTION OF HYDROGEN

Pure hydrogen has the best energy-to-weight ratio of any fuel (disregarding nuclear energy). It has however, the lowest volumetric capacity of energy storage as a gas at atmospheric pressure, which makes storage and distribution particularly important issues. Final applications, cost-effectiveness, and safety considerations are conditioning the most adequate technologies. The panoply of scenarios makes the topics challenging with plenty of possible technologies to be either improved or newly developed.

3.1. Hydrogen storage

The main available methods to store hydrogen include compression or liquefaction, adsorption, or in chemical forms (Züttel 2004). Storage technologies need to be analyzed in the context of large-scale transport and distribution, as well as for specific stationary or on-board final applications.

At present, local hydrogen distribution usually relies on trucks carrying hydrogen either as a gas or liquid, and this is likely to remain the case over the next years (International Energy Agency for the G20 2019). Hydrogen compression is a mature technology with high-pressure gas cylinders available up to 900 bar pressures. Although the liquefaction process is costly and hydrogen losses by boil-off are unavoidable, the technology and plants are currently operative. Actual costs for compressed H_2 represents 14.5 €/kWh (Rivard, Trudeau, and Zaghib 2019).

On a large scale, the geological storage of compressed hydrogen in caverns, and other underground reservoirs, is already being used. For a compressed storage at 200 bars, the electricity needs amount to 2.1% of the energy content in the stored H_2. Costs have been estimated at 0.91-2.73 € per kg of stored H_2 (Tarkowosk 2019). Geological storage could be associated to pipelines, which are likely to be the most effective long-term choice for local hydrogen distribution. Blending a progressive percentage of hydrogen into the current natural gas grid is possible, although a dedicated H_2 grid is necessary if the hydrogen is going to be used in PEM fuel cells. These grids would act as a large and low-cost source of storage capacity themselves.

Ammonia or liquid organic hydrogen carriers (LOHCs) are chemical storage alternatives, which are suitable for shipping and very long distance transport, with more convenient volumetric and gravimetric storage capacities (International Energy Agency for the G20 2019; Niermann et al 2019). Formic acid, methanol, cycloalkanes or organosilanes have been proposed at different levels of technology readiness (Niermann et al 2019; Aakko-Saksa 2018).

For stationary smaller scale applications, such as localized green hydrogen storage or isolated power/buildings supplies, a high volumetric capacity can be provided by solid hydride storage tanks (Gallandat et al 2017). Volumetric densities for metal and complex hydrides are around 150 kg H_2/m^3, while for high-pressure gas cylinders they are below 40 kg H_2/m^3, and for liquid hydrogen around 70 kg H_2/m^3 (Züttel 2004). Reversible (charging and discharging) tanks can already be found on the market based on chemical bonded hydrides.

For mobile/on-board applications, both high volumetric and high gravimetric capacities are needed. Available tanks made of lightweight composite cylinders filled with compressed H_2 at 800 bars can reach a gravimetric capacity of ca.13 (given as H_2 mass %) (Züttel 2004). Actual compressed hydrogen tanks at 700 bar have a higher energy density than lithium-ion batteries, thus enabling a greater autonomy in cars or trucks than that possible with batteries in electric vehicles. Costs for high-pressure tanks in on-board fuel cell electric vehicles (FCEVs) are 13.7-18.3 €/kWh.

Adsorbed hydrogen in large surface area materials (i.e., porous carbons or metal organics frameworks MOFs) is also a technology under consideration when operated at cryogenic temperatures and moderate pressures, typically -80°C and 100 bar.

Impact in basic science panorama and potential applications

From the above-described state of the art, it is clear that multidisciplinary basic science and engineering are needed to assess optimized hydrogen-storage technologies. Consider, for example, the multidisciplinary aspects covered in large-scale geological storage (Tarkowosk 2019).

Another example is how the fundamental physical-chemical knowledge of a broad variety of metal and complex hydrides (Sakintuna, Lamari-Darkrim, and Hirscher 2007) has been used to exploit the phase transition in metal hydrides to develop thermally driven metal-hydride compressors (Gallandat et al 2017). Moreover, well-established know-how in catalysis has been incorporated to develop the concept of liquid hydrogen carriers such as ammonia and LOHCs organic compounds (Aakko-Saksa 2018; Gallandat et al 2017).

Alternative methodologies are continuously under investigation for hydrogen-storage applications, such as clathrates, porous ice or white graphene. The chemical oxidation of metals (e.g. Li, Na, Mg, Al, Zn) with water (Bergthorson 2018), or the hydrolysis reaction of complex hydrides (e.g. sodium borohydride) (Demirci 2018), produce a liberation of hydrogen which is not directly reversible. The development of electrochemical reconversion processes with renewable electricity will lead to potential applications.

Investment in research programs to acquire new basic knowledge is needed to assess what storage is likely to be required in the future. New and improved options need to be considered in terms of volume and weight, duration, price, speed of charge/discharge, and energy consumption (Andersson & Grönkvisit 2019).

Key challenging points

1. For compressed hydrogen: improved materials and cost reduction for insulation and work at high hydrogen pressures; new magneto-caloric compression processes; safety issues.
2. For underground hydrogen storage: establish national inventories of underground caverns suitable for hydrogen storage. Prove the feasibility of hydrogen storage in depleted oil and gas fields as well as aquifers.
3. For cryogenic storage and liquefaction of hydrogen: improve the efficiency of the liquefaction process to reduce energy losses to below 30%. Reduce boil-off through improved insulation of the vessel as well as increased pressure levels. Develop liquid hydrogen pipelines (for example for handling in airports or in hydrogen refueling stations).

Increase energy density for on board LH2 storage for trucks, ships, trains and aircrafts.

4. For solid hydride materials: materials development for metal-hydride compressors (hybrid system); thermodynamic and kinetic improvements in reversible hydrogen storage from the gas phase and heat-management improvements.
5. For porous and nanostructured materials: novel nanomaterials design, hybrid materials combining ad- and ab-sorption.
6. For liquid carriers: catalyst development (low Pt content), cost effectiveness and durability. Catalytic processes improvements for conversion-reconversion.

3.2. Distribution

The use of hydrogen as an energy vector not only demands an efficient and cheap storage, but also requires its delivery at the demand points, under similar premises.

Three main transport possibilities are available nowadays: gas pipeline infrastructure, shipping and terrestrial (trucks/railways) (International Energy Agency for the G20 2019). A first possibility considers the blending of a small percentage of hydrogen into the current natural-gas grid. It could be considered an intermediate step toward a non-carbon economy. It nevertheless has some drawbacks, mostly related to the physical and burning properties of the mixed gas, which differ from those of the original natural gas. Moreover, natural gas should be eventually discounted in a real green hydrogen economy.

Terrestrial and maritime transport is expensive and faces the problem of the low gas density of hydrogen under standard conditions, which is related to the storage difficulties mentioned in the previous section. For transporting, several possible options among the ones shown in the previous section are, nowadays, in a sufficiently advanced technological state: metal hydride storage, compressed hydrogen (CGH2), liquefied hydrogen (LH2), ammonia (NH_3) and liquid organic hydrogen carriers (LOHC). NH_3 and LOHC can be transported by pipe-lines, technologically simpler than those necessary for hydrogen. Shipping of NH_3 and LOHC is also simpler compared to the other options, although empty return journeys increase costs for LOHC. NH_3 is the most developed for intercontinental transportation. Metal hydride current technology cannot compete in this aspect with the previous carriers. It has the added problem of the complex thermal management for conversion-reconversion of H_2. Methanol

TABLE 1–Cost of long distance transport and conversion, including intermediate storages, in Euro/kgH_2. Hydrogen is transported as a gas in pipelines (indicated by brackets). Conversion for H_2 is only needed if liquefied. Source: International Energy Agency for the G20, 2019.

	LH2			NH3			LOHC		
DISTANCE (KM)	1000	2000	3000	1000	2000	3000	1000	2000	3000
PIPELINE	(0.7)	(1.3)	(2)	0.4	0.6	1.1	0.4	0.6	1.1
SHIPPING	1.	1.2	1.3	0.2	0.2	0.2	0.2	0.2	0.2
CONVERSION		0.9			0.9			0.4	

TABLE 2–Cost of local distribution and reconversion expressed in Euro/kgH_2 Costs of hydrogen transported as gas indicated in brackets. Source: International Energy Agency for the G20, 2019.

	LH2			NH3			LOHC		
DISTANCE (KM)	150	300	500	150	300	500	150	300	500
PIPE 100 TPD	(0.3)	(0.5)	(0.8)	0.2	0.3	0.5	0.2	0.3	0.5
PIPE 500 TPD	(0.1)	(0.2)	(0.3)	<0.1	0.1	0.2	<0.1	0.1	0.2
TRUCK	0.2(0.7)	0.3(1.1)	0.4(1.6)	0.2	0.3	0.4	0.3	0.5	0.7
REC. CENTRALIZED		0			0.6			0.9	
REC. DISTRIBUTED		0			0.9			1.9	

needs carbon dioxide sources, which are difficult to find near renewable production, and the technology for extracting atmospheric carbon dioxide is too expensive. These two last options are neglected in this study. In all cases, a combination of shipping, terrestrial and/or pipe-line requires new or modified infrastructure, conversion-reconversion plants and storage at loading and receiving terminals. Transportation costs are briefed in Tables 1 and 2.

For long distances (Table 1), shipping transportation for NH_3 and LOHC always compares favorably to pipelines, even for short distances. For hydrogen (liquefied in ships, gaseous in pipelines), shipping is more competitive beyond 1500 km. These prices also include any storage required, but not conversion-reconversion and local distribution. Regarding local distribution (less than 500 km, see Table 2), adapted tanker trucks can be used for every hydrogen carrier. Pipelines (H_2 gas) may also be used for this range of distances. Using pipe-lines for LOHC and NH_3 is cheaper. Given the infrastructure required, and as indicated above (section 3.1), trucks will mostly be the main method for H_2 distribution in the near future. Regardless of the means of transportation, hydrogen reconversion adds an extra cost (Table 2), while LH2 and CGH2 are ready for use. In the case of NH_3, these costs could be saved if used directly in fuel-cells. Finally, it is important to note that in the case of some LOHC, the carrier has to return to the load point.

The total cost must take into account all the stages in the supply chain and possible synergies with other processes and existing infrastructures. There are also various technologies involved with different grades of maturity, which may evolve differently in the future, implying a different cost evolution.

An important issue to be considered is the cost of setting a net grid of hydrogen refueling stations (HRS) to provide fuel to FC vehicles. The average capacity station ranges from 100 kg/day to 350 kg/day, with infrastructure costs ranging from 1.9 M€ to 3.2 M€. These costs reflect early market, real-world conditions for the largest network of hydrogen fueling stations in North America (California Energy Commission 2015). It should be noticed that from the previous figures, overall hydrogen prices are much higher than the competitive price of natural gas, estimated at 1.4 €/kgH_2.

Impact in basic science panorama and potential applications
Hydrogen transport is closely linked to hydrogen storage. Any scientific/technological achievement in H_2 storage can substantially affect H_2 transportation optimization.

Specific impacts in the basic-science panorama still exist, related to the key challenges shown in the next section. For example, adaptation of existing gas infrastructure to H_2 distribution, in particular pipelines, may have an impact in material science. Analogously, the design of a functional and economic pressurized supply system for HRS would benefit from research in fluid engineering and thermal science.

Key challenging points
1. Due to its small molecular size, H_2 requires pipelines made of non-porous materials, such as stainless steel, which is quite expensive. Costs can be reduced by adapting existing gas ducts containing porous steels which, if not modified, suffer embrittlement from the diffusing hydrogen. Finding an adequate coating or some chemical treatment to adapt high pressure gas pipelines to H_2 use is a key challenging point. Adaptations for the low-pressure gas (plastic) pipelines and ancillary materials, such as valves, manifolds, etc, are also needed.
2. Regarding refueling in HRS, there are some open challenges about the best configuration (in situ H_2 generation by electrolyzers vs external

input) and the improvement of the pressurized supply system (compressors), in particular the thermal aspects (chiller).

3. Other specific challenges are related to energy conversion and transportation logistics. This last aspect is general to a great variety of goods.
4. For energy conversion, some interesting scientific/technological changes are open. Direct production of ammonia from renewable sources and NH_3 direct fuel cells (better at low temperatures) would avoid the need of conversion-reconversion from H_2. Reverse fuel cells would be ideal. Research in direct fuel cells for other H_2 alternative carriers is another interesting challenge.

4. HYDROGEN UTILIZATION

For years, hydrogen has been mainly used in the industrial sector, but its potential growth in the medium- and long-term is considered to be high. Considerable growth is also expected in both residential and transport sectors when fuel-cell technologies are widely used in combined heat and power (CHP) units and fuel-cell hybrid electric vehicles (FCEV). In addition, the use of hydrogen in both centralized or decentralized approaches can potentially enhance energy-system flexibility providing new links between energy supply and demand.

4.1. Hydrogen in the industrial sector

The top four single uses of hydrogen (in both pure and mixed forms) in the industrial sector are: oil refining (33%), ammonia (27%), methanol production (11%), and steel manufacture via direct reduction of iron ore (3%) (International Energy Agency for the G20 2019). Europe has a major petrochemicals and chemicals industry that produces about 15% of the total global refining and chemicals output, demanding 325 TWh of hydrogen as feedstock every year. About 95% of the hydrogen used in these industries currently comes from natural gas by SMR without CCS or byproduct. Consequently, over 35 Gt of CO_2 are emitted worldwide every year, and this figure will inevitably increase considering the tendency of both economic and population growth (International Energy Agency 2018).

Oil refining

Hydrogen is primarily used in refineries to remove impurities (e.g. sulfur) from crude oil and to upgrade heavier fuel oil using both hydrotreatment and hydrocracking processes. Hydrogen is also used to upgrade oil sands and to remove oxygen from vegetable oils and animal fats that are processed into biodiesel. Today, the consumption of hydrogen for oil refining reaches 33% (38 MtH_2/yr) of the total global demand in refineries, emitting 230 $MtCO_2$/yr.

Chemical industry

The production of ammonia and methanol constitute the second- and third-largest sources of demand for hydrogen today with a rate of 31 MtH_2/yr and 12 MtH_2/yr, respectively (Bruce et al 2018). The chemical sector also manufactures other products such as plastics, fertilizers, solvents and explosives (ethylene, propylene, benzene, toluene and mixed xylenes) and high-value chemicals (ethane, liquefied gas and naphtha), which raises overall demand to 46 MtH_2/yr. It is also used to produce synthetic fuels in the chemical industry (methane, methanol, liquid fuels) when combined with CO_2 in thermochemical (methanation) processes or Fischer-Tropsch synthesis.

For years, fossil fuels have been a cost-effective source of hydrogen for ammonia and methanol production, emitting around 630 $MtCO_2$/yr. Although most of the technology and equipment required for CO_2 capture in the chemical sector are already available, low-carbon ammonia and methanol production today is not yet cost-competitive. The total levelized production cost for methanol varies from 370 €/t for unabated natural gas to 500 €/t when CCS is considered, and up to 1190 €/t when hydrogen is produced by renewable electrolysis. In the case of ammonia, cost varies from 550 €/t to 760 €/t and up to 1740 €/t, respectively (IRENA 2019).

Iron and steel industry

Over three-quarters of global steel production occurs by primary conversion of iron ore to steel, known as direct reduced iron (DRI). In 2018, global steel production reached 1809 Mt, emitting 2532 tons of CO_2 [13]. To this end, the sector needs around 4 MtH_2/yr of dedicated hydrogen production as a reducing agent in DRI via the iron-electric arc furnace (DRI-EAF) route and, in contrast, 9 MtH_2/yr of hydrogen by-product that is mostly combusted in the blast furnace-basic oxygen furnace (BF-BOF) pathway. A technical option that is now being promoted is the direct injection of ammonia as fuel in BF-BOFs, which does not generate CO_2.

Considering current dynamics, steel production is projected to grow around 2% by 2030. Thus, the DRI-EAF route could supply 14% of primary steel demand, requiring 8 MtH_2/yr. To reduce CO_2 emissions from primary iron and steel production, both "CO_2 avoidance" strategies using hydrogen as the reducing agent, and "CO_2 management" pathways with the direct application of CCS to traditional fossil fuel-based routes, are now under development.

Hydrogen for high-temperature heat

Industrial high-temperature heat (IHTH, > 400°C) is required in processes such as melting, gasifying, and in chemical reactions. It is principally employed in the chemical and iron, steel and cement manufacture sectors. Demand is predicted to rise continually. Currently, fossil fuels are the principal source of IHTH, although electricity is widely employed in electric arc and induction furnaces. IHTH is responsible for ~ 3% of global energy-sector CO_2 emissions (International Energy Agency for the G20 2019). Although scarcely used at present, combustion of sustainable bioenergy or hydrogen is an effective way to reduce emissions of large-scale processes (Bruce et al 2018). Nevertheless, hydrogen is an expensive low-carbon pathway for the energy system, even when CO_2 prices reach ~100 € /tCO_2. Bioenergy tends to be more cost-effective than hydrogen-based fuels and may become competitive with natural gas for IHTH in 2030. However, hydrogen can help to decarbonize the market in areas where CCS is difficult. The importance of hydrogen may also increase if the supply of sustainable bioenergy is curtailed due to high demand for bioenergy from other sectors.

Impact in basic science panorama and potential applications

Several actions must be undertaken to reach the 2050 decarbonization target established by the Paris Agreement. Firstly, the technical and economic feasibility of electrification and use of biomass to replace fossil fuels with renewable electricity, as well as the development of innovative processes (e.g., electrochemical production processes), should be explored. Secondly, CCS technologies must be extensively employed in dedicated facilities where hydrogen is produced from fossil fuels, but focusing on the use of electrolytic hydrogen obtained 100% from renewable energies for most industrial processes.

Key challenging points

1. To adapt technological processes and equipment for the progressive replacement of natural gas with ultra low-carbon hydrogen (electrolysis 100% from renewable sources) in most industrial processes, including DRI plants for steel processing.

2. To fully replace fossil-fuel feedstock with hydrogen and CO_2 from biomass in the production of hydrocarbon-based chemicals such as methanol and derived products to create so-called “CO_2 negative emissions” scenarios.
3. To cost-effectively scale up electrofuel production, allowing the energy produced from all renewable sources as liquid fuels to be conveniently stored.
4. To achieve commercial-scale iron reduction using ammonia to produce cost-competitive steel in regions with relatively high production costs of ultra low-carbon hydrogen.
5. To develop advanced monitoring and combustion control technologies, as well as new burners, adapted to the combustion characteristics of hydrogen flames (high combustion velocity, non-luminosity and corrosiveness).

4.2. Hydrogen for transport

Transport emissions from road, rail, air and marine transportation, account for over 32% of CO_2 emissions in the EU, and they are expected to grow at a faster rate than that from any other sector. Hydrogen fuel cell electric vehicles (FCEVs) can reduce pollution, as they have no tailpipe harmful emissions. Moreover, hydrogen can be converted to hydrogen-based fuels and synthetic liquid fuels (“power to liquid”) taking advantage of existing infrastructure.

In road transport, the short refueling time, less added fuel weight and zero exhaust emissions of FCEVs could translate into a lower material footprint than lithium batteries. Although passenger FCEVs currently have a higher cost of transport than internal combustion engines and battery electric vehicles, it is expected that FCEVs could reach parity around 2025 (International Energy Agency for the G20 2019).

Railway is presently the most electrified mode of transport. Hydrogen and battery electric trains represent an excellent alternative for replacing non-electrified trains, and are most cost-effective for rail freight employed in regional lines with low network utilization (International Energy Agency for the G20 2019).

International shipping is an important contributor to climate change, deteriorating air quality in and around ports. Since maritime freight activity is expected to grow significantly, 2050 greenhouse-gas targets could promote the use of hydrogen-based fuels, with ships serving long-distance maritime trade routes offering the greatest opportunity. Nevertheless, storage costs and space for hydrogen is higher than for other fuels, requiring the redesign of ships, shorter distance trips and more frequent refueling.

Aviation was responsible for ~ 2.8% of worldwide CO_2 emissions in 2017, and air-passenger traffic is expected to double by 2050, requiring alternative fuels to mitigate emissions. The scope for using hydrogen in small planes is currently limited to small demonstration projects and requires significant investment in R&D. Conversely, hydrogen may also be used in APUs (auxiliary power units) in large aircrafts, saving approximately 20% of aircraft emissions at airports and during taxiing (International Energy Agency for the G20 2019).

Impact in basic science panorama and potential applications

The target in the transport sector is to eliminate about 72% of CO_2 from the EU transportation fleet by 2050, equal to roughly 825 Mt. To this end, R&D investment in FCEV technologies is ongoing, requiring improvement in electrode efficiencies, better component inter-compatibility and durability, and lower material costs. The biggest cost reductions for FCEVs are expected to come from the establishment of automated, dedicated production lines and manufacture of FCEV-specific components at scale. Until the global demand for mass vehicles is established, strategic pilot projects are likely to play an important role in stimulating uptake of FCEVs, by providing the initial infrastructure and demonstrating the usability and safety of FCEV technologies.

Key challenging points

1. A massive shift in scoping the transportation system is required which involves development of highly efficient hybrid powertrains and alteration of the value chain for FCEVs easing the transition from oil to renewables.
2. Production of low-cost and high-performance membrane electrode assemblies for polymer electrolyte membrane (PEM) fuel cells by replacing noble-metal electrocatalysts and developing new membrane materials.

4.3. Hydrogen in stationary applications

Hydrogen can be used as fuel in stationary fuel-cell systems for buildings, backup power, or distributed generation. In the building sector, energy efficiency can be increased by using the waste heat from the co-generation of power and heat. For example, stationary fuel cells are proposed as an ideal solution for decentralised electricity generation in off-grid areas using micro co-generation systems. In combined mode, i.e. electrical and thermal, stationary fuel cells can achieve efficiencies of up to 95%, while the electrical efficiency is around 45% (Fuel Cells and Hydrogen 2 Joint Undertaking 2019a). In particular, they are becoming gradually more important as emergency power supply (EPS) or uninterruptible power supply (UPS) systems. The backup capacity of stationary fuel cells varies from a few kW to several MW. Around 3,000 fuel-cell-based UPS systems were employed in 2018. In addition to generated electricity, the produced heat could also be used in households in combined heat and power (CHP) units. To this end, stationary PEMFCs or SOFCs up to 10 kWe are typically employed. This application is particularly interesting for SOFCs, as the existing natural-gas infrastructure can be used. The use of CHP systems for the domestic sector is growing rapidly around the world, especially in Korea, Japan, and Europe. The current FCH 2 JU funded PACE project aims to install at least 2,500 units in Europe by 2021, as part of a manufacturing transition to higher volumes in the order of 10,000 units/year post 2020 (Pathway to a Competitive European 2020).

Impact in basic science panorama and potential applications

Even though demonstration projects for stationary applications are in continuous development, basic research is still needed to reduce materials and cell costs of current fuel-cell systems. Potential applications include the use of UPS systems for data centres, banks, hospitals and similar organizations. This is a potential route for both PEMFC and SOFC to scale up, and will significantly reduce costs (the initial cost per kW has come down by 75%, from more than 32, 100 € to 8, 250 € in 10 years) (International Energy Agency for the G20 2019). Another target application includes the use of fuel cell-based CHP systems in isolated houses, blending hydrogen into the natural-gas grid. A blending hydrogen level of 5% could save about 200,000 tons of CO_2 annually (International Energy Agency for the G20 2019).

Key challenging points

1. Reduce present costs of PEMFC by reducing the amount of Pt on the electrodes and finding alternatives to Nafion©.
2. The main challenge for SOFC technology is to achieve performance and reliability at a cost consistent with wide spread commercialization. Metal-supported cells offer the possibility of lower costs. Development of new materials is still required, especially Cr resistant cathodes. The use of standard materials in new engineered designs and morphologies

(by 3D micro-patterning, infiltration or exsolution) presents significant potential to address these issues.

3. Promotion of CHP demonstration projects in order to establish fuel-cell micro-cogeneration technology in the market.
4. In the short term, to adapt or substitute current natural gas boilers and heat pumps for hydrogen boilers, as part of the transition to future CHP systems.
5. In the medium-long term, strengthen projects to introduce hydrogen and ammonia as fuel for gas turbines and coal power plants, in order to use the surplus renewable electricity.

4.4. Other applications

Portable fuel cells offer significant weight advantages over rechargeable batteries and generators. Some portable fuel-cell applications include laptops, cellular phones, power tools, military equipment, battery chargers, unattended sensors, and unmanned vehicles (ground, aerial and underwater). They can also provide small-scale emergency power and are particularly useful in areas where grid power is unavailable. In addition, utility vehicles (forklifts, airport movers, wheelchairs, or small military robots) have been a successful early adopter of fuel-cell technology as they currently use lead-acid batteries, which require maintenance and long charging times (Compendium of Hydrogen Energy 2016). Portable fuel cells can also provide reliable, high-quality power in non-emergency situations, such as remote construction sites.

Impact in basic science panorama and potential applications

As commented, fuel cells for portable applications have several niches for potential uses. However, cost reduction (mainly by reducing catalyst loading and manufacturing), greater efficiency (by reducing fuel crossover and increasing catalyst selectivity), and reduction in the size of the hydrogen storage system are still required.

Key challenging points

1. To promote the use of fuel-cell forklifts in Europe, as the total ownership cost is projected to decline around 30 per cent by 2050.
2. In the short-medium term, to boost the use of fuel cells for unmanned aerial vehicles, improving the flight time and shortening refueling times.
3. To increase the use of fuel cells in power systems for portable electronic equipment in the military market.

5. REGULATION, CODES AND STANDARDS

Looking into new hydrogen scenarios, such as energy or sustainable mobility, from the point of view of policymaking, regulation and legislation frameworks, most laws have to be defined, passed and adopted by the legislative bodies at European, national and regional level, to ensure their correct impacts. What is more, new standards and codes or review of existing ones have to be established in order to provide rules and guidelines for the proper practices in these emerging contexts.

New ways of low- and zero-emission production from renewable energies, mainly by means of electrolysis processes, must be boosted taking into consideration the legal frameworks as well the final use of the hydrogen produced, the daily amount made or the need for storage and transport to fulfil requirements. In this regard, Guarantees of Origins procedures must be taken into consideration (CertifHy 2016). Moreover, new forms of hydrogen transportation such as a gas/liquid (LOHC, NH_3...) have to be taken into account in these upcoming frameworks, as well as by large maritime vessels, and storage in sites including existing gas stations and new hydrogen refuelling stations. In addition, the green origin, quality and purity (to avoid damage to the fuel cell) of this hydrogen have to be assured, as well as procedures to validate the correct measurement of hydrogen supply in hydrogen refuelling station are some considerations in the mobility sector. Furthermore, hydrogen as an alternative fuel is not reflected in the existing hydrogen industrial-focused regulations. Therefore, adaptation and the creation of new regulations, including the new hydrogen applications for sustainable mobility, infrastructure and vehicles, are mandatory (Hylaw 2018).

Hydrogen will be a key actor in the future energy economy, totally or partially replacing natural gas, but also substituting combustion engines or boilers with new technologies based on fuel cells (Plan director del Hidrógeno en Aragon 2020). Using the existing infrastructure to transport hydrogen and couple with existing sectors, conditions of usage and access have to be facilitated. In addition, fiscal and incentivising legislation has to be established and existing regulatory barriers have to be overcome to create a suitable scenario in which decarbonation solutions become widespread (Fuel Cells and Hydrogen 2 Join Undertaking 2019b).

5.1. Conclusions and recommendations

Existing regulations and normative related to hydrogen are totally focused on the industrial and chemical sectors. Applications in the energy sector require adaptation and establishment of new, specific regulation. Without a proper legal structure, the potential emerging market will be developed at a slower pace.

With the creation of proper guidelines, barriers along the whole value of chain of hydrogen will be lifted, unleashing the development of new energy hydrogen applications (GRTGaz 2019).

Ensuring the green origin of hydrogen is fundamental to exploit all the foreseen benefits. Downstream, the transportation of hydrogen thorough new distribution paths will define new certifications and requirements for vehicles, especially considering hydrogen may be transported as gas or liquid. Likewise, procedures for the implementation of hydrogen refuelling stations will require new regulation for land use designated for their construction, redefinition of the legal requirements and consideration of all the environmental, technical and personal safety aspects.

Finally, as regards hydrogen injection in the existing natural gas infrastructure, the legal framework status must involve the regulatory authorised bodies and consider the variation of hydrogen concentration levels in the high-pressure gas-transmission system with proper technical, quality and safety requirements. In addition, reinforcement of the monitoring and metering infrastructure have to be carried out to ensure safe operation of both the grid and the end-user equipment, involving the allocation of costs and incentives related to this new scenario.

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TABLE 3—List of challenges to be addressed for the Challenge 8

	NEAR TERM (< 5 YEARS)	MID TERM (5-10 YEARS)	LONG TERM (10-20 YEARS)
PRODUCTION	• Natural gas steam reforming with carbon capture and storage (CCS). • Integration of the electrolysis electrical grid.	• Autothermal reforming of natural gas with CCS. • Coal Gasification with CCS. • Biomass Gasification with CCS. • Reforming of biomass-derived liquids. • Dry reforming of biogas. • Improvement of durability and sustainability of the materials for low temperature electrolysis.	• High temperature electrolysis. • Thermochemical cycles. • Direct water splitting using sunlight. • Microbial biomass conversion.
STORAGE AND DISTRIBUTION	• Pressurized tanks. • Hydrogen pipeline/delivery system in industrial clusters. • Hydrogen Refueling Stations (HRS).	• Green ammonia initial production. • Liquid organic hydrogen carriers (LOHC). • Improved Hydrogen Refueling Stations (IHRS). • Hydrogen pipeline to connect production sites with demand centers. • Innovative advances in other technologies: metal hydrides, porous high surface area materials, chemical oxidation of metals with water, large geological storage.	• Liquid organic hydrogen carriers (LOHC) from CO_2. • Green Ammonia improved electrochemical devices • New hydrogen storage materials
USES	• Refining. • Ammonia production. • FCEVs for light-duty vehicles, busses, ships and trains. • Hydrogen boilers for combined heat and power.	• Demonstration of iron ore reduction using hydrogen for steel. • Methanol production. • High-grade heat. • FCEVs for heavy-duty trucks, trains, and ships. • Unmanned aerial vehicles. • Military equipment.	• Gas turbines. • Variety of vehicles.

	NEAR TERM (< 5 YEARS)	MID TERM (5-10 YEARS)	LONG TERM (10-20 YEARS)
REGULATION, CODES AND STANDARDS.	• Hydrogen purity requirements for its different application. • Certify origin of green hydrogen. • Review gas pipeline regulations to consider including gaseous hydrogen. • Regulatory framework for wider implementation of hydrogen storage. • Implement regulations that provide appropriate compensation for grid firming services from electrolysis.	• Refueling station regulations.	• Robust hydrogen code at international level.

ONE SLIDE SUMMARY FOR EXPERTS

Challenge

Considering that energy-related CO_2 emissions account for two-thirds of global greenhouse gas emissions, an alternative carbon-free energy power is required for the deep decarbonization of current energetic system based on fossil fuels and avoid the undesired CO_2 emissions. Hydrogen, as an energy carrier, is a clean and storable solution that could decarbonize several economic sectors presently based on fossil fuels. Thus, hydrogen is being considered a serious alternative by the automotive, chemicals, oil and gas, and heating industry to achieve their sustainability objectives.

Approach

Hydrogen is not an energy source, is an energy carrier and then, energy is needed to generate pure hydrogen. That means that hydrogen can have a significant carbon footprint depending on the primary energy source and the process used for its production, and need to be considered when quantifying climate benefits. Then, classical technologies for hydrogen production based on steam reforming of natural gas are being implemented with CO_2 capture and storage (CCS) technologies to produce low emission hydrogen. New catalytic materials with improved robustness and lifetime to produce hydrogen from biomass by reforming/gasification are being also studies. Sustainable production of hydrogen using solar and wind energy by water electrolysis, thermal cycles and direct water splitting using sunlight are also being investigated. For hydrogen storage, several methods to store hydrogen at higher energy densities are being developed: compressed or liquefied, adsorbed and/or in chemical form. Distribution and transport of hydrogen is available nowadays using gas pipeline infrastructure, shipping and terrestrial (trucks/railways). Considerable growth is expected in both residential and transport sectors when fuel-cell technologies are widely used in combined heat and power (CHP) units and fuel-cell hybrid electric vehicles (FCEV). Hydrogen can also be converted into electricity in combustion systems (internal combustion engines or combined-cycle gas turbines) or in power-to-gas-to-power technologies (combining electrolyzers and fuel cells). The use of hydrogen in both centralized or decentralized approaches can potentially enhance energy-system flexibility providing new links between energy supply and demand.

Social and economic impact

Hydrogen technologies and fuel cells can deliver, on the one hand, societal and environmental benefits, and on the other, jobs creation and positive economic impact. The hydrogen economy offers a great opportunity to support high quality jobs, which will require highly skilled and trained workers, as well as excellent opportunity to turn our natural energy resources, including renewables like biomass, solar and wind energy, into a uniquely low-emissions energy product, providing energetic independence and increasing the local, regional and national wealth.

Involved teams

Several groups of different Institutes of the CSIC are working in the development of hydrogen technologies in order to build a more sustainable hydrogen economy, help meet agreed emissions targets and address concerns around energy security. These Institutes are: ICB, INCAR, ITQ, LIFTEC, ICMA, ICP, IRII, CIN2, ICV, ICMM, ICMS, IDAEA, ICTJA, ISQCH, ICTP, and IMB-CNM.

ONE SLIDE SUMMARY FOR THE GENERAL PUBLIC

Challenge

Hydrogen in the most abundant chemical element in the Universe. It is a versatile energy carrier and feedstock that can enable deep decarbonisation across the energy and industrial sectors.

Hydrogen is a very appropriate element for intermittent renewable energy that requires a clean and efficient storage system. All these qualities, especially security of supply, efficiency and zero emissions, make hydrogen a very promised fuel to face the need to reduce CO_2 emissions.

Approach

Hydrogen is not an energy source, is an energy carrier and then, energy is needed to produce it. Currently the most important route to produce hydrogen is through the use of natural gas, a fossil energy source, being directly accompanied by CO_2 generation. Thus, to realize the full benefits of hydrogen as fuel, hydrogen should be produced from available renewable energy sources (e.g. biomass, solar and wind). Different process and technologies are being developed to increase the efficiency in the hydrogen production from renewables (e.g. gasification of biomass, electrolysis, etc), to decrease cost production and to avoid CO_2 emissions.

Hydrogen can also provide storage options for intermittent renewable energy sources such as solar and wind. It can be converted to energy (heat) either through combustion or through an electrochemical reaction in the called fuel cells devices to generate heat and electricity in an efficient way and can be used in stationary or mobile applications. Thus, hydrogen holds the potential to provide energy services to all sectors of the economy such as transportation, buildings and industry.

Social and economic impact

Hydrogen technologies and fuel cells can deliver, on the one hand, societal and environmental benefits, and on the other, jobs creation and positive economic impact. The hydrogen economy offers a great opportunity to support high quality jobs, as well as excellent opportunity to turn our natural energy resources, including renewables like biomass, solar and wind energy, into a uniquely low-emissions energy product, providing energetic independence and increasing the local, regional and national wealth.

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CHALLENGE 9

SOCIAL AND ENVIRONMENTAL ASPECTS OF THE ENERGY TRANSITION

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1. INTRODUCTION AND GENERAL DESCRIPTION

The need to promote a swift, efficient and fair energy transition to clean, secure and efficient energy production, storage, transport, and consumption is a major challenge for the future of the planet (EC 2020). Currently, massive emissions of greenhouse gases (particularly CO_2) and other pollutants are changing global climate, and the lasts report of the Intergovernmental Panel on Climate Change (IPCC 2018) advised that keeping the temperature increase below 1.5 ºC will require drastic, urgent and internationally coordinated actions. These initiatives will greatly affect advanced economies, characterized by high energy consumption, which should seek for clean and secure local energy sources, but they are also highly relevant for quickly developing countries, whose biodiversity, natural resources and standards of living are at risks due to over exploitation of local resources or to accumulation of waste products of energy production technologies coming from elsewhere. These processes of transition, though, have generated a variety of social and environmental impacts and, at the same time, have triggered complex questions about sustainability and social acceptance (i.e. Sánchez-Zapata et al. 2019 for wind and solar energy production in Spain). Social and environmental aspects of the transition to clean, secure and efficient energy production, storage, transport, and consumption should then be fully incorporated into research on new energy sources to ensure its sustainability.

2. IMPACT IN BASIC SCIENCE PANORAMA AND POTENTIAL APPLICATIONS

Several sources of energy production have engaged in highly sophisticated technological transitions to reduce costs, improve efficiency, reduce environmental impacts and carbon footprint, and increase the economic advantages of a transition to renewability. Solar, wind, hydro-derived, biomass and hydrogen, to mention but some reviewed here, have largely improved their outputs, efficiency, costs and profitability over the past two decades. As reviewed in the other chapters, these technological developments have profited from strong investment in both basic and applied research both in Spain and all over the world. Potential impacts of these technological developments on societies and on the environment have, however, lagged behind, in spite of its importance to ascertain whether such developments were truly sustainable (i.e. Morales-Reyes et al. 2015). Basic approaches aimed to integrate technological developments with social and environmental issues are thus of upmost relevance at present.

3. KEY CHALLENGING POINTS

The key social and environmental issues that research and development of new energy sources must tackle can be summarized in five main points:

3.1. Efficiency and control of energy demand

No energy source, either traditional or new, can fully cover demands if control of energy requirements is not taken into account. The quest for a clean, cheap and inexhaustible energy source that would solve humankind problems has long been given up within the field of science fiction.

Substantial reductions in both greenhouse emissions and energy demands can be achieved by improving energy efficiency. For instance, buildings are responsible for approximately 40% of EU energy consumption and 36% of the CO_2 emissions, and a huge share of this consumption is lost through floors, roofs, windows, doors and walls (Dall'O 2020). Further, the construction sector is on its critical path to decarbonise the European economy by 2050, reducing its CO_2 emissions by at least 80% and its energy consumption by as much as 50%. However, the inherent characteristics of the chemistry of cement pose certain limits to the achievable reduction. On the other hand, investments in energy-efficient new buildings, and in the improvement of the current ones, will have much impact not only in reducing the consumption of energy, but also in the creation of new jobs and business areas, many of them of high technical level. Therefore, both social and economic benefits are envisioned through the expected decrease in energy consumption and the incorporation of new industrial high-level activities.

Further savings can be achieved by promoting *in situ* production systems whenever possible, such as small-scale solar panels or wind turbines placed at consumption sites (i.e. buildings, housing developments, small towns), or developing energy-scavenging technologies (see below). *In situ* production will also reduce energy losses during transport, together with developing technologies for the production of superconductors working at not too low temperatures, as well as environmental impacts of transport lines (loss of landscape values, wildlife causalities, pollution; i.e. Sánchez-Zapata et al. 2019). Disperse, small-scale production systems will reduce the amount of land and resources needed per unit of energy production, thus facilitating the integration of productive uses in multifunctional systems of land use (Budischak et al. 2013). Small distributed systems produce lower environmental and social impacts than large infrastructures of production, storage and transport (i.e. large dams, large-scale biomass crops, solar and wind fields, or transport power lines). Nevertheless, large-scale energy centrals and large renewable production plants are more amenable to optimization, and most likely, will be still be necessary for important industrial goals in the mid-term. Effort to integrate the impacts of these centrals and their associated transport structures, and the ways to deal with them efficiently, will be needed to maintain the needed social support to these infrastructures.

Increasing the use of electricity in the demand-side can play a vital role in mitigating climate change provided that it comes from low CO_2-emission renewable energy sources in the supply-side (solar, wind, biomass). Mobility and climate control in buildings sectors are showing a significant development in this way, although the industrial sector has shown a relatively slow transition rate towards more electric solutions (Sugiyama 2012). Taking into account the importance of the sector as energy consumer (25-30% of the total energy consumption), energy savings in the industrial sector and increased use of renewable energy sources have ample room for sustainability-oriented innovation. This point has been recently addressed in large-scale policies, though.

In this sense, it is pertinent to think about how to project future energy consumption from the humanities and social sciences. Current studies on social impact have focused on job opportunities provided by renewable energies, on the efficiency of their practices and on the necessary combination of different policies to support them. But all these research projects start from the same premise: that energy consumption levels can only increase in the future. These papers consider that economic growth will be continuously increasing, and suggest that the role of new technologies will be to help make that growth as sustainable as possible. Every day more machines, shipping containers, infrastructure elements, vehicles and people are being equipped with networked sensors to report their status, receive instructions and even take action based on the information they receive. There are an estimated 22 billion connected devices worldwide, including smartphones and computers. Over the next decade, this number is expected to increase dramatically, with estimates reaching up to 50 billion devices in 2030 (Statista 2020). However, in the near future there could be another scenario. The Covid-19 pandemic has shown how power consumption can change and experience a profound reduction, although at the expense of huge socioeconomic costs. The advent of a global economic crisis could nevertheless promote a restructuration of economic systems to adjust and accommodate new social needs that may not be based on accelerated economic growth, but on other ways of a fair distribution of resources. If the economic system changes, the energy transition processes, will also have to change.

No clear cue for the time scale of this likely change is currently available. For this reason, behaviours related to energy consumption -both individual and domestic consumption, as well as consumption by industry and commerce, transport or public services- should be one of the main focuses of social research in the context of energy transition. Traditionally, studies on technology and innovation have been focused on the design of technologies. But in recent years there has been a growing interest in that R. S. Cowan has called "consumption junction", or the ways in which users make choices about technologies, based on shared information, values, and attitudes and/or social and cultural meanings (Cowan 1987, Zachmann 2002, Bakardjieva 2006).

Quantitative and qualitative studies on energy consumption would allow:

1. Knowledge on the ways in which users interact with technologies and the interpretations they make of different energy sources.
2. Understand the dynamics of consumption and their articulation in the context of sociotechnical systems, to identify possible conditioning factors for energy overconsumption and the barriers to its reduction. These behaviours related to energy source choices and decreased consumption is an essential part of the success of any sustainability strategy.

3.2. Renewability, duration and recyclability of energy sources

Even though control of demand is key for developing truly sustainable energy production systems, most current research deals with the reduction of CO_2 emissions responsible of the climate crisis. Smart grids (see below) are intermediate approaches aimed at combining control of demand, efficiency, and renewability. Decarbonisation of the economies and, more generally, independence from scarce and unevenly distributed resources such as fossil fuels, radioactive minerals or rare earth elements, is the key driver of energy research (EC 2020). Within this paradigm, renewable energy sources using durable and/or recyclable materials, or systems to recycle waste coming from traditional energy sources, are investigated. Apart from economic reasons derived from independence, it is assumed that renewable sources will have no (or at least less) negative environmental and social impacts. Comparatively fewer work is being done on whether this assumption is true and on how to improve it, however.

Despite its interest for the fossil fuel industry, it is widely recognized that the deployment of technologies for large-scale Carbon Capture and Storage (CCS) and Carbon Capture and Utilisation (CCU) is not currently in the mainstream of research. Nevertheless, the large imbalance between what is really needed in most scenarios to reach a maximum 1.5ºC increment in 2050 vs what is positively perceived by the public and policy-makers is a paradox that requires increasing research attention from social science. Transparent, honest, unbiased, fact-based scientific knowledge needs to gain more prominence into public policy on climate change. Safety concerns related to the permanent storage of CO_2 and environmental side effects of any large new infrastructures for capture, transport and storage of CO_2 hinder acceptation of CCS strategies, since despite the limited risks reported (Vilarrasa & Carrera 2015) the scale of this alternative for significant effects is huge and hence difficult to accept. However, disruptive and unpopular technological solutions such as CCS may be necessary in the long term to stabilize the climate because the long lifetime of CO_2 in the atmosphere does not lend for a quick decline of atmospheric concentration, even if a significant decrease on emission is promptly achieved. CCU has received much more support from the public within the framework of circular economy and 'negative emission' concepts based on CO_2 capture by biomass, despite their inherent larger cost and high energy and resource inefficiencies (i.e. vast requirements of renewable energy inputs and/or constrained biological resources). CCS and CCU technologies are however essential to decarbonize the industrial sectors most addicted to carbon (i.e. cement, ceramics, metal, C-containing chemicals, etc.; IPCC 2018). Besides, CO_2 capture from atmosphere, despite being technological and economically challenging, may be necessary to reduce atmospheric CO_2 concentrations as quickly as needed. Further, combining these approaches with the use of sustainable resources such as geothermic or biomass, and the advances in other technologies such as catalysis and electrochemical hydrogen production may even revert net carbon balances to the negative side.

Using biomass to produce heat, electricity and transportation liquid biofuels holds much promise for providing renewable energy sources. The need to have a continuous and significant supply of biomass bring about many other positive effects, including the recovery of degraded lands that cannot be used for other purposes, improved production of oxygen due to intense photosynthetic activity of fast-growing trees, decreased erosion of cultivated soils when compared to degraded pasture lands, or improved soil coverage with organic matter from the forest. In some cases, the need for more lands for plantation of energy crops may compete with land used for food and feed production, therefore, there is also a need to promote the production of bioenergy and biofuels based on alternative sources such as lignocellulose waste (as cereal straws), algae or forestry residues.

Pollution derived from use of fossil fuels combustion (i.e. NO_x) can also be reduced by new catalytic technologies. Although pollution produced by terrestrial transportation can be addressed by a shift to electrical modes, emissions of greenhouse gases to the atmosphere by the industry and other transport means (i.e. airplanes) will increase unless transformed and/or processed efficiently. In addition, catalytic processes could come to the rescue of a planet with an excess of carbon in the atmosphere: capture and transformation of CO_2 into fuels or commodities, using renewable electricity or direct sunlight, is possible with catalysts; catalytic processes may become more and more selective, so that less residues (especially carbon-containing ones) can be generated; fuel cells and electrolysers involving better electro catalysts will be more efficient. This research line, linked to research in safe and efficient energy storage systems, will be key to translate renewable energy production to the transport system, which is responsible for a large share of pollution derived from energy consumption (Ritchie & Roser 2017). Research in new catalysts and batteries should be directed towards the use of recyclable components rather than on mining, as recycling reduces carbon footprints. Efficient storage can also facilitate decarbonisation of transport through its electrification if energy sources are renewable, a fact that requires Life Cycle Assessment (LCA) analyses.

Renewable energy is the backbone of efforts aimed at mitigating climate change. The production and transportation of renewable energy (hydroelectric, solar, wind-based, biomass-based) has, however, potentially severe environmental impacts on wildlife and landscapes. Hydroelectric production is probably the most impacting one as it affects many ecological processes (flow regime, habitat alteration, biological invasions) and wildlife populations, but this impact is not exclusive of hydroelectric infrastructures, being shared with those devoted to irrigation, urban and industrial water supply or other uses. Wind energy production is an emerging source of environmental impact at both local and regional scales. Land wind farms produce habitat destruction as well as alterations in the microclimate. Perhaps the most striking impact is the mortality of vertebrates, known for decades, and which has been quantified from population approaches in many studies worldwide. Finally, solar facilities impact mostly at the local scale through habitat alteration and loss, water consumption, and the use of hazardous materials in manufacturing but can vary greatly depending on whether technology is based on photovoltaic solar cells or concentrating solar thermal plants. The construction of solar facilities on vast areas of land imposes clearing and grading, resulting in soil compaction, alteration of drainage channels and increased erosion whereas central tower systems require consuming water for cooling, which is a concern in arid settings. Their effects on wildlife have been, however, little studied, although vertebrate mortality can be high. If concentrated in solar or windmill fields, as it is usual, these sources of energy share the need for transportation by means of power lines that have significant negative effects on wildlife. The expansion of renewable energies is a very recent phenomenon, so that pre-installation studies on potential impacts are usually of low predictable power. In spite of legal requirements, investigations on impacts lack appropriate statistically powerful experimental designs such as the Before-After-Control-Impact (BACI) to help isolate the effect of the development from natural variability. There are national and European guidelines for the consideration of the impact on birds and bats of wind energy projects. There is currently enormous variability and, in general, lack of rigor, in the field studies aimed to monitor the environmental impact of these infrastructures. Currently, research on the ecological impact of renewable energies is led in Spain by CSIC teams. It seems advisable to strengthen the lines already existing in the CSIC that focus on ecological effects of renewable energies on vertebrate populations.

Hydrogen technologies will play a key role in the future decarbonized economy. Life Cycle Assessment (LCA) of pros and cons of these technologies seems promising. More interestingly, the LCA approach can help selecting among different alternatives of energy production according to needs. Harmonization of LCA methodologies is then essential.

Efficiency of energy production may be boosted by technologies for micro energy scavenging, that is, for powering smart devices by recovering energy from lights in offices, random movements of the body or from small changes in temperature. Coupling geothermal energy sources with thermoelectric ones could be also promising. These technologies can provide energy for wireless sensor networks monitoring environmental conditions within buildings, cities and large constructions in a remote and sustainable way, avoiding battery recharging, or even replacing them. Thus, the development of energy scavengers to potentially work at micro and macro scales will have a huge environmental, technological and economic positive impact with a valuable contribution to achieving Europe's sustainability ambitions. Energy harvesters may provide self-powered wireless sensor networks for monitoring buildings, human health, and environment or be used as an auxiliary power source for portable, wearable electronics, a market to reach 75 billion devices in 2025. Over 20% of industrial energy input is lost in vibrations and variable temperature fluctuations, scavenging of even a fraction of this lost energy would have a transformational environmental and economic impact. Besides, progress in multi-source scavenging, exploitation of 1D materials, nano structuration and eco/friendly materials will strengthen the strategic position of European scientific activities in KETs' (Horizon Europe). Integration of energy scavenging with local production and control of demand by means of efficient and intelligent electric grids (aka Smart-Grid) will be crucial to allow bidirectional flow of electric power and information. Smart-Grids will play a main role in coupling the requirements from the use-side (for example, industry) and the production-side (for example, intermittent wind and solar sources). These networks, as mentioned above, could be further promoted through the Internet of Things, a tool that is still in the early stages of growth. Nevertheless, important issues regarding the use and control of the big data generated by these widespread technologies has to be solved before its full implementation, to avoid excess control of devices by a handful of powerful corporations.

Explicit consideration of the environmental effects of different new energy sources though Life Cycle Assessment (LCA) of positive and negative effects would allow:

1. To concentrate efforts in the more promising technologies from the point of view of renewability and efficient use of materials
2. To integrate energy production with other societal demands regarding climate change prevention, biodiversity conservation and pollution minimisation

3.3. Social impacts: economy, safety, health and training

Social acceptance is key for a technological project to prosper. New energy sources, although traditionally demanded by society, have not been exempt from opposition and public debate either. To try to understand the resistance against these technologies and expand social trust in them, the CSIC should work in three directions: think of procedures by which to channel information and make inquiries that favour citizen participation; try to become interlocutors and not opponents to collectives and organizations that question them; and work to introduce these topics into official study programs.

The accumulated knowledge, from studies on social innovation to those of the philosophy of science and technology, indicates that one of the social challenges that the transition towards the generation of clean energy would be to study holistically the procedures in order to understand the dynamics of acceptance-rejection by society, as is being done with hydrogen technologies. Social Life Cycle Assessment (SLCA) is being proposed as the key methodology to assess social impacts along the value chain of a product. Its guidelines were defined by UNEP/SETAC in 2009 (Benoît & Mazijn 2009). SLCA follows the methodology of LCA, but taking into account that the social conditions of each country involved in the supply change has a deep influence in the social impacts of the product. Therefore, the geographical scope is key in SCLA.

Hydrogen technologies and fuel cells present different transversal barriers, not only related to social acceptance; safety and training should be taken into account, too. The general public will be the main recipient of these applications in the sector of sustainable mobility and stationary applications for building. Therefore, it is key to spread hydrogen technologies, increase their positive perception in all terms -especially safety- and promote the inclusion of hydrogen technologies in curricular itineraries. More specialised audiences such us stakeholders, technicians and mechanics will need to be equipped with hydrogen-technology skills.

But the introduction of training programs at universities and other training institutions is not unique to hydrogen technologies. It is a common challenge in this period of energy transition. All these new technologies will require a new generation of engineers and qualified personnel with technical profiles which, not being available at present, will demand new actions to the academic establishment and training schools to adapt their current curricula. In addition, not only industry will require of these new personnel, but also the services and even finance sectors will demand new personnel with expertise in the field and capacity for control assessment, consulting and certifying. Therefore, several training programs on all of these renewable technologies must be defined and included at different levels of official studies.

Social acceptance does not only go through safety and training, it also has to take into account people's health. For example, while the low-carbon industry will improve air quality, reduce pollution, and predictably also social problems related to the possible or perceived effects on workers' health, increased exposure to electromagnetic fields in massively implanted electrified industries will require studies to investigate possible health effects. This is a controversial topic, still relatively little explored, and where contrasting results have been found (Sidaway 2008, INTERPHONE Study Group 2010, Barron & Torero 2017).

Last but not least, there are the economic impacts. There is abundant literature on this matter, especially related to solar photovoltaic energy and wind off-shore power, showing that the high costs of support for renewable energy in the past may have also influenced its social acceptance. But there are other economic barriers to these technologies that have rarely been explored, such as the impacts of markets on supply chains, which would open up an interesting field for designing policies that lead to their mitigation. In this sense, auctions seem to be crucial and alternative instruments to put renewable energy on the markets. Auctions promoted by the European Commission pose an interesting socio-economic challenge: designing policies that show society that renewable are efficient and profitable. Right now, its cost is very competitive compared to its fossil-fuel competitors (EC 2020). Thinking about the effects that the deployment of renewable energy could have on employment is another interesting challenge that could also have a greater social acceptance of these technologies (IRENA 2019). In this sense, it would be interesting to know what types of jobs they would generate and where they would be located.

The different conflicts and synergies generated in this period of energy transition require complex policies that try to balance social conflicts and mitigate them. In this sense, analyses from economics and political science have a lot to add as well (Kiefer and del Río 2020).

Integrating social acceptance into the energy transition would imply three major tasks:

1. Promote studies on social perception.
2. Assess the media discourses that appear on energy in the mass media. This analysis can help frame and contextualize energy issues and reflect on the narratives that society incorporates and why.
3. Improving scientific communication to the general public. Quality scientific communication contributes to the scientific culture of citizens and their ability to form opinions and make decisions about the different ways in which energy issues affect their lives, on a daily basis and in the long term. The social communication of science can be carried out by the researchers themselves, by specialists in scientific communication, and also by the administration. In any case, it requires responsibility, honesty, transparency and impartiality of the person who communicates; this scientific communication must always be based on scientific facts and recognizes the uncertainties and limitations of different technologies.

3.4. Multifunctionality of landscapes

Renewable energies are going to have, in fact they are already having, a profound influence on society. These technologies modify physical landscapes - windmills and large photovoltaic fields are good examples - but they also modify economic and industrial landscapes. These technologies allow us to think of a decentralized generation and management of energy, a circumstance that would change rural landscapes.

We know that the use of more domestic energy sources will improve the security of energy supply and make local economies less vulnerable. Maybe the best example on how industrial electrification could provide a combined secure energy and industrial production supply is electrification through electrolysis of water and the use of hydrogen and hydrogen-rich feedstock and fuels (Philibert 2019). Hydrogen technologies are in fact considered as the most efficient way to solve problems derived from the intermittent production of energy of most renewable sources, specially wind and solar. But there are other examples. The use of biomass to produce liquid biofuels for heat, electricity and transport opens up a promising space for providing a local source of renewable energy that can be a viable alternative to fossil fuels. However, safety concerns and environmental issues of, respectively, hydrogen and biofuels can hinder the rapid deployment of these technologies.

The biofuel industry could revitalize the development of rural economies. Energy crop plantations can be attractive to homeowners and small farmers seeking a safe return on investment. This return would allow them to diversify the use of their land, increase their profitability, and thus create jobs and provide other services to their region. This new source of income can reduce dependence on government aid. On the other hand, a continuous and significant supply of biomass would result in the reuse of degraded lands that are no longer used for agriculture and livestock. Nevertheless, biomass production should be integrated with other agricultural and forestry goals such as food production and environmental protection; ways to design and evaluate this integration are however available since relatively long (Díaz & Concepción 2016).

Decarbonisation processes have also caused recent changes in landscapes. Many territories have gone through these processes to lessen the impacts that these industries have on climate change. But they have sometimes been poorly understood socially, mainly due to problems related to permanent storage of CO_2. But in the face of the environmental benefits that decarbonisation has, it would also be necessary to consider other social aspects, such as the abandonment, aging and depopulation of these territories. In this sense, it would be interesting to think of strategies that allow, on the one hand, conserving and reusing the knowledge and practices related to this form of energy and, on the other, to safeguard that industrial heritage in a rapid process of loss.

In this sense, catalysis has important social implications. For example, depending on the minerals and metals required by the catalysts, it may be necessary to open new mines and close others that have become obsolete. Also, non-catalytic materials needed for photovoltaics, windmill engines, batteries, electronics, even for new facilities transforming biomass, may require new mines. This will not only impact landscapes, it will also impact employment by destroying some jobs and generating others. This process can be well appreciated in the chemical industries: the outdated ones will disappear, while new business opportunities related to renewable energy and green chemistry will emerge and create new jobs.

Incorporating new energies to multifunctional landscapes would imply:

1. Consider landscapes not only as physical spaces; also, as social, economic and industrial spaces.
2. Convert the technological changes that are taking place in the different territories into strengths and new opportunities.

3.5. Fair and equitable access to energy

Justice and energy sovereignty are central themes of contemporary democracies. Research on new energies has as one of its most important social challenges to allow and promote fair and equitable access. In this respect, among the sustainable development priorities established by the United Nations, the point SDG N.7 considers the access to affordable, reliable, sustainable, and modern energy for all (https://sustainabledevelopment.un.org/). For example, a critical issue is how the energy transition in general and the costs and benefits of promoting renewable will impact different segments of the population. In particular, although the costs of key solar and wind renewable electricity technologies are already relatively low on private costs alone (levelised electricity costs), the substantial increase required in these technologies and the costs that their variability imposes on the electricity system may increase the costs for electricity consumers and aggravate energy poverty problems. The extent to which this will be so will depend upon the degree of increase of those costs as well as the adoption of mitigation policies for the most vulnerable segments of the population.

Humanities and Social Sciences have an important role in this field with the identification and management of energy justice problems that may arise from innovations in the production, distribution, storage, transport and consumption of new energy in this scenario of energy transition. Examples of this importance are research to develop batteries that do not require rare earths to prevent international conflicts over source sites and pollution derived from the use of non-renewable or scarcely recyclable energy sources. The CSIC does not have specific research groups on this topic, although at the Institute of Philosophy there are researchers who work on social justice in other areas.

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ONE SLIDE SUMMARY FOR EXPERTS

Challenge

The energy transition towards clean, secure and efficient energy use is a major challenge for the future of the planet (EC 2020). This transition involves a variety of social and environmental impacts that may compromise its sustainability and social acceptance. Social and environmental aspects should then be fully incorporated into research on new energy sources to ensure its sustainability.

Approach

- Statistically powerful experimental designs such as the Before-After-Control-Impact (BACI) design, including pre-installation measurements, to fully evaluate, mitigate, and prevent, impacts on the environment.
- Harmonized Life Cycle Assessment (LCA) of technical advantages and disadvantages of available alternatives of energy production according to needs and environmental impacts.
- Social Life Cycle Assessment (SLCA) of alternative sources, taking into account the social conditions of each country involved, and seeking for integration of production and consumption systems at local scales within multifunctional landscapes.
- Widening SLCA to world scales to ensure fair and equitable access to energy.

Social and economic impact

Ensuring that new systems of energy production, storage, transport, and consumption are truly clean, secure, efficient and sustainable will be a major step towards a more equitable and fair human society. Dissemination and education of true facts and rigorous life cycle assessments will ensure social and economic support of these new energy systems and promote a swift transition from traditional energy sources that have proven to be unfair and dangerous for the health of both people and the environment.

Involved teams

Only a couple of groups within the CSIC are specialised in evaluating socio-economic and environmental impacts of new energy sources, and concentrate their efforts within the narrow field of wind power energy. They are at the Estación Biológica de Doñana (environmental impacts) and at the Instituto de Políticas y Bienes Públicos (socioeconomic impacts). Several individual researchers in both humanities and environmental institutes have partially worked on topics related to the integration of new energy developments within societies and landscapes. Collaboration between these people and groups focused on technological developments is necessary. Only the work of multidisciplinary teams can guarantee the development of new truly sustainable energy sources.

ONE SLIDE SUMMARY FOR THE GENERAL PUBLIC

Challenge

The energy transition towards clean, secure and efficient energy use is a major challenge for the future of the planet. This transition involves a variety of social and environmental impacts that may compromise its sustainability and social acceptance. Social and environmental aspects should then be fully incorporated into research on new energy sources to ensure its sustainability.

Approach

- Launch experimental facilities to carry out prior evaluations of technologies and thus, more effectively, mitigate and prevent social and environmental impacts.
- Evaluate alternative energy source in each stage of the processes -production, storage, transport, consumption- to know, jointly, the advantages and disadvantages they offer according to societal needs and environmental impacts.
- Evaluate alternative energies taking into account the socioeconomic conditions of the countries.
- Integrate energy production and consumption systems with other land uses (food production, recreation, research) within multifunctional landscapes.
- Evaluate and guarantee fair and equitable access to energy.

Social and economic impact

Making the new energy production, storage, transport and consumption systems truly clean, safe, efficient and sustainable will be an important step towards a more equitable and fair human society. The communication of research results and the training of citizens will ensure greater social and economic support, that will result in a rapid transition and a gradual abandonment of traditional energy sources.

Involved teams

Only a couple of groups within the CSIC are specialised in evaluating socioeconomic and environmental impacts of new energy sources, mostly regarding the rapid development of wind power energy in Spain. Several individual researchers in both humanities and environmental institutes have partially worked on topics related to the integration of new energy developments within societies and landscapes. Collaboration between these people and groups focused on technological developments is necessary. Only the work of multidisciplinary teams can guarantee the development of new truly sustainable energy sources.

The impact of energy production by conventional technologies on the environment and human health has promoted transition policies towards a new model for the energy sector. In this context, it is essential to identify the key challenges which favour the global implementation of a clean, safe and efficient energy system, focused on the ways in which energy is produced and stored, and the management of existing resources and their emissions.

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