The role of Carbon Capture, Utilization and Storage (CCUS) on the pathway to Net Zero greenhouse gas emissions: can we accelerate the transition to a low-carbon economy?

El papel de la captura, almacenamiento y usos de CO_2 en el camino hacia cero emisiones netas de gases de efecto invernadero: ¿podemos acelerar la transición hacia una economía baja en carbono?

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The world is currently facing unprecedented times due to the COVID-19 pandemic, where we are heading for a steep recession triggered by the outbreak and expected to be worse than the 2008 financial crisis. After this crisis, the time will come to rebuild our social and economic systems and we have there the opportunity to restart growth in a greener era. The current COVID-19 situation did not make the climate crisis disappear (**Figure 1**), even though in many countries the most striking and clearly visible effect of COVID-19 was a dramatic decrease of pollution levels. If we can indeed rebuild our society under a green social and economic recovery scenario, i.e., fighting climate change and promoting biodiversity, we will rebuild stronger and more sustainable economies. Furthermore, the transition to a climate-neutral economy has the potential to rapidly deliver jobs, growth, and to contribute to building more resilient societies. At the European level, calls for a Green recovery were getting louder, and in some countries COVID support to industry has been conditioned to a more sustainable operation. It seems then clear that rescue measures should advance the EU's landmark Green Deal policy package, which aims to meet the goal of getting to net zero greenhouse gas emissions by 2050.

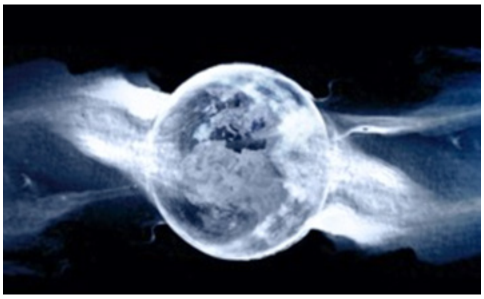

Figure 1. The world's ever-expanding CO_2 emissions (Credit: Luke Robus and Emmet Norris)

Carbon Capture, Utilization and Storage (CCUS)

Carbon Capture and Storage (CCS) is a key technology for achieving global greenhouse gas emissions reduction targets because of its role in power and industrial decarbonization. It is a proven technology that involves three steps: 1) capturing (i.e., separating) carbon dioxide, CO_2, from combustion flue gasses and gas streams produced by industrial plants; 2) the compression and transport of CO_2, and: 3) its safe storage in underground geological formations [1]. If instead of storing the CO_2 we use it as a carbon feedstock for different applications, such as the production of synthetic fuels or chemicals, then we are talking about Carbon Capture and Utilization (CCU) technologies. CCS and CCU have been often seen in the past as competing technologies and it has become evident over the past years that we need all the help we can get in order to achieve our net zero targets, hence the CCUS concept. One only needs to make sure that for every fossil fuel carbon atom we take out of the ground, we put one CO_2 molecule back, as otherwise we will never be achieving the net zero concept. CCUS technologies can reduce emissions across most existing industrial and energy facilities. But we do not need to stop here, we can also remove CO_2 from the atmosphere, either together with bioenergy or as Direct Air Capture [2]. It is widely acknowledged that the lowest cost and risk approach to achieve net zero emissions requires a broad portfolio of technologies and strategies, and not implementing CCUS would significantly increase the mitigation costs (by 29%-297%) [3] that we need to pay.

The Challenge and the Opportunity

To achieve our net zero targets, decarbonization from a variety of industrial emission sectors will be required, which highlights a marked need for capture technologies that can be optimized for different sources of CO_2 and integrated in an equally diverse range of applications of captured CO_2 as a feedstock (**Figure 2**).

At high Technology Readiness Levels (TRLs), there are substantial efforts focusing on optimizing a single particular carbon capture technology (e.g., amine-based capture) for a single typical stationary source (e.g., natural gas-fired power plants). However, significant gains in energy efficiency and other economic benefits can be obtained if we tailor make a capture technology for a particular CO_2 source

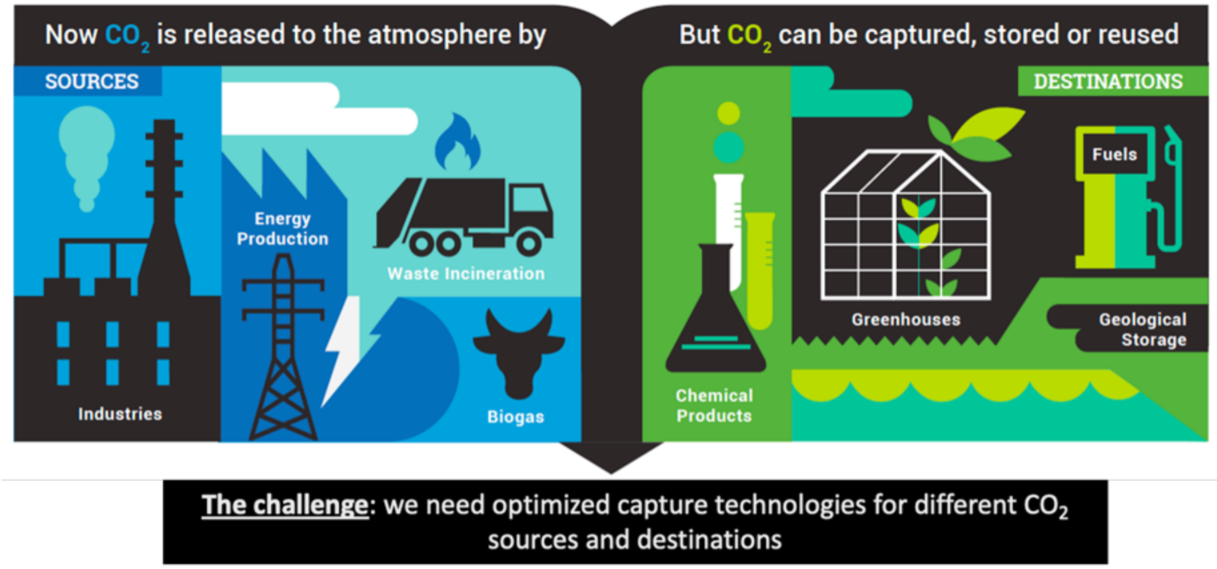

Figure 2. Schematic with examples of CO_2 sources and destinations

(e.g., waste incineration, coal combustion, cement manufacture) and a particular CO_2 destination, such as utilization or transport via pipeline, or ship to permanent storage. This offers the opportunity for more innovative CO_2 capture technologies that are currently at low TRLs, i.e., sorbent-based ones, to breakthrough into current markets and provide the required flexibility together with reduced capital and operational costs. It is precisely this vision towards achieving zero anthropogenic CO_2 emissions, the one that drives the research of my team.

My research group at Heriot-Watt University ambitions to change the paradigm on how novel processes based on advanced materials are developed through the integration of process engineering and basic science. At present, there is a significant gap of knowledge, which is often referred to as the "Innovation Valley of Death", that hinders the realization of many novel promising materials beyond lab scale testing. Our approach integrates Chemical Engineering with Data Science, Computational Chemistry, Materials Science and Chemistry to synergistically deliver that integration in Open Access platforms. An example of this approach was our breakthrough on the computational design of new materials that can capture CO_2 from wet flue gasses better than current commercial ones [4].

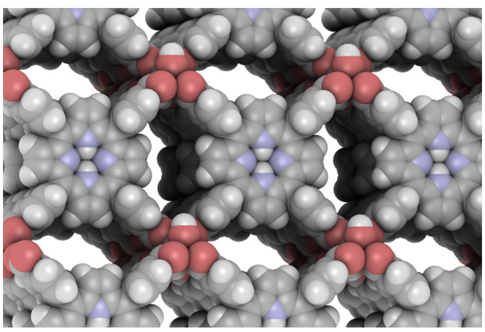

Figure 3. A molecular representation of a MOF carbon capture material (Credit: M. Moosavi and K. Jablonka; iRASPA software was used for visualisation)

This work got inspired by drug design tools used by the pharmaceutical industry, where common motifs, i.e., structural properties, are established for those molecules that bind successfully to a target protein. These common features form then the basis for designing and synthesizing actual drug molecules. By applying the same concept, we identified, out of a database of 325,000 computer-generated sorbents, those whose common motif was the ability to bind CO_2 but not water. All the materials in the database belonged to the family of Metal Organic Frameworks (MOFs) [5], which are highly versatile porous crystals that are made from combining metal nodes with organic linkers (**Figure 3**). Selected identified top-performing materials (**Figure 4**) were further synthesized, characterized and tested under mimicked real industrial operation, and results showed that our predictions were correct.

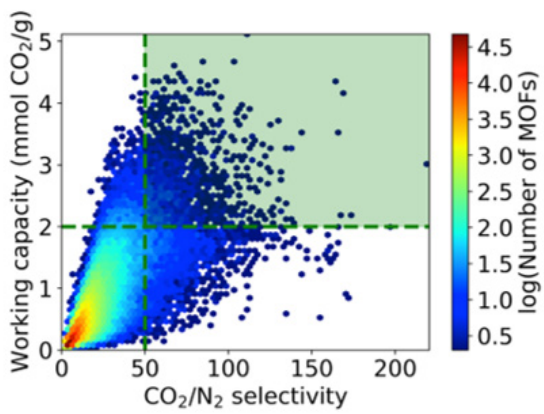

Figure 4. Computational screening of MOFs for strong CO_2 adsorption and selectivity

International collaboration as a key factor for accelerating CCUS technologies

Our current research builds up on the abovementioned efforts and aims to accelerate the transition of energy and industrial sectors to a low-carbon economy by developing a technology platform to tailor make cost-efficient carbon capture solutions for a range of different CO_2 sources and CO_2 use/destinations.

To achieve this aim, we have secured support from the European Union's highly competitive ERA-NET Accelerating CCS Technologies (ACT) Program to lead an innovative and ambitious three-year project, as part of a joint bid with academic and industrial partners from across Europe and the USA. The ambition of ACT is to facilitate the emergence of CCUS via transnational funding aimed at accelerating and maturing CCUS technology through targeted innovation and research activities.

The awarded ACT-funded PrISMa project (Process-Informed design of tailor-made Sorbent Materials for energy efficient carbon capture) received a total funding of €3.3M, and it unites the efforts of world-leading research teams from Heriot-Watt University (HWU) in the UK, École Polytechnique Fédérale de Lausanne (EPFL) as well as Eidgenössische Technische Hochschule Zurich (ETHZ) in Switzerland, Lawrence Berkeley National Laboratory (LBNL) in the USA, and SINTEF Energy Research (SINTEF-ER) in Norway. These teams have the expertise to bridge the gap between molecular sciences (LBNL and EPFL) and process engineering (ETHZ, SINTEF-ER and HWU). The consortium is supported by market-leading companies and non-governmental organizations, which are committed to minimize CO_2 emissions of their industrial sectors and provide case studies and maximise knowledge exchange and impact of PrISMa.

The PrISMa methodology (Fig. 5) starts with a high-level analysis, in terms of an effective carbon price, on how the performance of a separation process depends on the source of CO_2 and its use/destiny. This analysis is subsequently translated into key performance indicators (KPIs) that novel materials need to achieve in terms of their potential to reduce the effective carbon price in order to compete with state-of-the-art capture processes. A materials genomic approach [6] is used to screen libraries of millions of *in silico* predicted structures to identify materials that meet the KPIs. The most promising materials are then synthesized, characterised, and tested for their performance in a carbon capture process. For those materials that yield a significant reduction of the effective carbon price, a roadmap to bring these materials to TRL5 will be developed through case studies.

PrISMa provides the platform needed for high-throughput screening of materials to maximise their impact, to enable the design of efficient pilot-scale test facilities with improved processes under real conditions and, to decrease the time to market of affordable, cost-competitive, low environmental impact, and resource-efficient advanced capture technologies. As a similar approach can be developed for other separations, we expect the impact of PrISMa in terms of the potential to decrease the time to market for novel materials to go beyond carbon capture. In addition, PrISMa aims to initiate a systematic thinking about efficient solutions to mitigate CO_2 emissions from different local CO_2 sources that are optimal for a specific local setting. In such a setting the impact of PrISMa will be significant as the need for tailor-made solutions will be increasingly important if CO_2 mitigation at the local level becomes the norm.

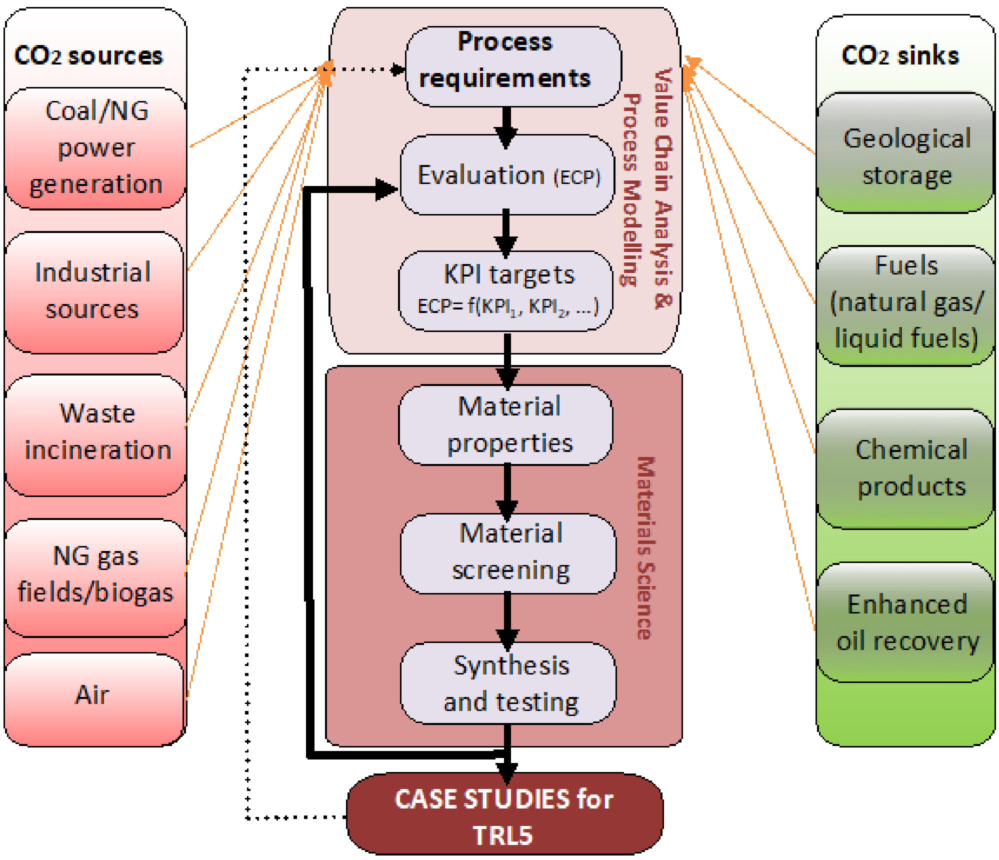

Figure 5. Illustration of PrISMa platform

Building bridges

This need for international collaboration and interdisciplinary approaches to tackle global challenges like CO_2 emissions to the atmosphere is now, more than ever, of striking evidence. Funding programmes all over the world as well as different societies and foundations are encouraging research at the global level, as well as knowledge transfer and research dissemination and outreach to the general public, as the basis for successful deployment and implementation of the required technologies to achieve net zero targets. As an example, and as the recipient of the Society of Spanish Researchers in the United Kingdom (SRUK/CERU) and Banco Santander Foundation Emerging Talent Award 2020, my goal is to create an awareness that our society needs to change into a more sustainable, equal, inclusive and diverse one.

As scientists, we are committed to drive the required research and innovation for a better society, and pushing forward the required transition to a clean sustainable energy is one of the key objectives of my research. The recognition and support from SRUK/CERU and Banco Santander Foundation provides me with the opportunity to encourage new international collaborations and strengthen the links between the Spanish and UK scientific community, to increase scientific culture in the public and act as an ambassador and inspiring reference for the role of women in Spanish science.

In a world where drastically reducing CO_2 emissions is one of our most urgent and important global challenges, we do need all the help we can get!

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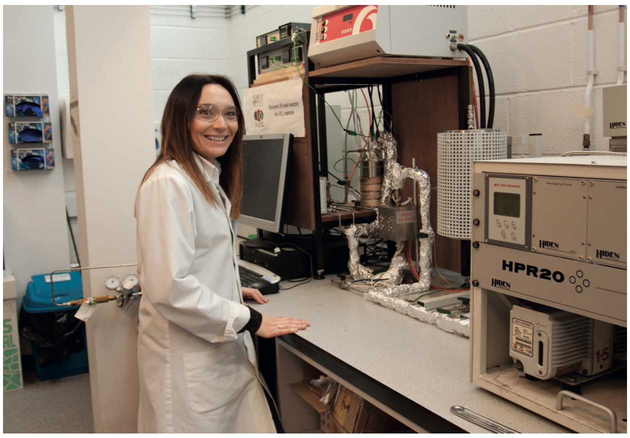

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