

DECEMBER 2022 |

NEWSLETTER

III EDITION

What is CO2MPRISE?

EU FUNDED PROJECT

CO2MPRISE is a project funded by the EU Horizon 2020 Research and Innovation Framework Program. It is within Marie Skłodowska-Curie Actions - Research Fellowship Program and Research - and Innovation Personnel Exchange (RISE).

Excellence training in solutions for CO2 capture technology aims to bring together subject matter experts from the academic and non-academic sectors to develop new technologies in CO2 capture and conversion field. The project's objective is to find an inexpensive, effective and robust solution for significant CO2 reduction from industries and civil transport, what represents one of the main and fascinating challenges proposed to the scientific community for the next 10 years. It is considered as a pillar of HORIZON2020.

CO2MPRISE aspires to reach these ambitious results through a common solid knowledge basis arising from a balanced number of secondments that guarantee a cross-sectorial synergy between recognized research centres, industry and academies.

Highlights

CONSORTIUM -
PARTNERS

LAST CONSORTIUM
MEETING

PROJECT ACTIONS

COMMUNICATION AND
DISSEMINATION:

- BEERS & BRAINS
- PRESS RELEASE

KNOWLEDGE
TRANSFER:

- MOOC FILMING

SECONDMENTS



This project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No 734873

UNISS | University of Sassari (Italy) – Project Coordinator

With over 18 thousand students and 700 teachers across 4 campuses, 11 faculties and 40 departments in Sassari, Olbia, Nuoro and Oristano, the University of Sassari (UNISS) promotes international courses and advance research projects with the active engagement of the local community and its global partners. Best “medium- sized” Italian university as stated by Censis Research Institute in 2009-10.

International programmes: i) Erasmus Programme which allows student exchange around Europe; ii) ULISSE programme for non-EU mobility opportunities iii) Erasmus+, or Erasmus Plus.

Department of Chemistry and Pharmacy is in charge of training fundamental and applied scientific research in various areas of Chemical and Pharmaceutical Sciences. It was founded in 2012 following the reorganization of the University that has provided training departments with teaching tasks and research. Research activities carried out at the Department are related to Organic Chemistry to Applied Physicist. High Education program for master students is provided by Ph.D. School in Chemical Science and Technology.

Since 2016, the Department of Chemistry and Pharmacy has activated an international Master Course jointly with the University of Wroclaw (SWIMINCHEM). In 2015-2016, in chemistry area, was published more than 200 international articles.

[Website](#)

UBU | Universidad de Burgos- ICCRAM (Spain)

UBU-ICCRAM is a privileged Research and Innovation core belonging to the University of Burgos, that constitutes an Excellence International Center in Critical Raw Materials in synergy with a Competence Center devoted to Advanced Industrial Technologies.

ICCRAM is a leader actor within the European Innovation Partnership in Raw Materials (EIP Raw Materials) taking part in 6 commitments and coordinating an strategic linking the future of EU Nanotechnology and Materials value chains to the efficient use and management of Critical Raw Materials. ICCRAM also leads the Critical Raw Materials Industrial and Resource efficiency Strategy in Castilla y Leon (Spain).

ICCRAM was born conceived to integrate within its structure an "intrinsic path into innovation", and it is supported by an industrial board of industries, SMEs and clusters. Moreover, it coordinates an industrial platform with the City Council in the context of transition into Circular Economy.

The main areas of research are: applied nanotechnology, ecocompatibility, nanobiotechnology, materials by design, new materials technology and new alloys; resource efficiency in industrial value chain of graphene technology, biotechnology and industrial production of resources, processing technologies and advanced materials synthesis lab.

[Website](#)



HZG | Helmholtz-Zentrum hereon GmbH (Germany)

HZG is a non-profit making research institute with limited liability. Its shareholders are the Federal Republic of Germany, the federal states (Länder) of Brandenburg, Hamburg, Lower Saxony and Schleswig-Holstein, the Gesellschaft zur Förderung des Helmholtz-Zentrums Geesthacht e.V. (Society for the Promotion of the Helmholtz-Zentrum Geesthacht) as well as a number of renowned companies.

The centre is based in Geesthacht, Germany. In 1992, the Working Group Teltow became a part of it. The Helmholtz-Zentrum Geesthacht is a member of the Helmholtz Association of German Research Centres.

The department of Nanotechnology works within the frame of the Helmholtz "Advanced Engineering Materials", programme carry out studies of nanostructured materials for hydrogen storage.

In addition, the possibility to produce such materials in a large-scale and to test it under application-oriented is investigated. Solid state hydrogen storage – based on light metal hydrides or hydride composites – enables us to create an extremely safe storage system for use in future zero-emission vehicles and in chemical energy storage.

[Website](#)



CNEA | Instituto Balseiro-Bariloche (Argentina)

The CNEA is the National Atomic Energy Commission (Comisión Nacional de Energía Atómica) dedicated to the peaceful development of nuclear energy. Balseiro Institute (University of Cuyo) is one of the bases of the CNEA, founded in 1955, and it is one of the most prestigious research centres in Latin America.

Balseiro Institute is the academic sector, where students study Physics, Nuclear, Mechanical or Telecommunications Engineering. It also offers advanced courses, international workshops and schools, PhD and Master programs open to all students in Argentina and the rest of Latin America.

On the other hand, the Bariloche Atomic Center is the research institution. Both are intimately linked since the students do experiments in the labs of the Centre and the professors are all active researchers there.

The nearly 200 researchers are mainly employees of CONICET (Consejo Nacional de Investigaciones Científicas y Técnicas) and/or CNEA. The objectives are to conduct research and development in the nuclear and non-nuclear areas; promote the scientific and technological activities and contribute with the formation of high-level human resources.

[Website](#)

MON | MONOLITHOS Catalysts (Greece)

Monolithos Catalysts is an SME industry in accordance with EU standards with highly qualified employees in branches of chemical engineering. Much of its annual turnover comes from exports, mainly to Germany. MON has extensive experience of more than 15 years in the manufacture, regeneration and recycling of catalytic converters. Its main activities are:

- Manufacturing of automotive emission control devices (catalytic converters and diesel particulate filters for passenger cars).
- Manufacturing of catalytic converters, diesel particulate filters (DPFs) and Selective Catalytic Reduction (SCRs) for heavy duty applications (off-road/trucks/buses).
- Regeneration of Diesel Particulate Filters and Selective Reduction Catalysts.
- Gathering, sorting, pre-processing and recycling of spent catalytic converters.
- Manufactures and regenerates catalytic converters and diesel particulate filters for mobile applications.

Within this project it focuses on the development of precious metal nanoparticles, replacing conventional precious metal molecules with precious metal nanoparticles in a catalytic wash coat and transition metals in a catalytic wash coat. It also develops ceramic monoliths using catalysts in its structure and hollow fibers to replace the ceramic honeycomb, between other actions.

[Website](#)

UCH | Universidad de Chile (Chile)

the University of Chile was founded in 1842, being the oldest institution of higher education in Chile. It is located in the capital city of Santiago de Chile and is a public university with international quality. All areas of knowledge are in the top of the Chilean university system.

The University of Chile has more than 40,000 students, divided into undergraduate and postgraduate studies and about 4,000 teachers. It is distributed in five campuses and several experimental stations in Santiago and other regions of Chile, with 14 different faculties. There are also 4 Interdisciplinary Institutes.

Also, several Chilean presidents have been students of the University of Chile, and the only two Chileans who received the Nobel Prize, Gabriela Mistral (1945) and Pablo Neruda (1971), both in Literature, were members of the University.

National prizes in different fields have been awarded to members. It is placed among the 400 best higher education establishments in the World Ranking of Universities, 10th place among its Latin American peers and first place in Chile in the Ranking of Research Institutes (SCIImago Research Group, Spain 2017).

[Website](#)

Last consortium meeting

OCTOBER 2022

Partners from all participating institutions came to the University of Burgos, Spain, to present the progress of their work packages and to bid farewell to the project after five years.

At the beginning of the meeting, the President of ICCRAM, Alfredo Bol, and the Vice-Rector for Research and Knowledge Transfer, José Miguel García Pérez, warmly welcomed all the attendees.

After that, Gabrielle Mulas, coordinator of the project from University of Sassari, started giving an overview of the project's achievements.





Project actions

2017 - 2022



Training, workshops and seminars have been planned with the aim to impart to each partner of this consortium the fundamental skills mainly based on the technical aspects, the social challenges involved in this sector, and last but not least, market capacity.

Particular attention has been also given to organize the strategy work of all activities in specific processes in order to finally introduce the results achieved into the international market.

In addition, scientific papers and patents have been developed in the project framework, as well as communication and dissemination actions like seminars, MOOC's or trainings.

Strategies

The scientific strategies regard the study of:

- i) Olivine-based materials to convert carbon dioxide to methane and test its potentialities under practical conditions.
- ii) Photocatalytic reduction of CO₂ by solar radiation.
- iii) The not-yet explored metal-hydrides, instead of hydrogen gas, to efficiently convert CO₂ to hydrocarbons in the Fisher-Tropsch reaction activated by mechanochemical input.
- iii) Robust, inexpensive and free-metal solid sorbent membrane based on multi-walled carbon nanotubes (MWNTs) and Graphene-based sorbents, for CO₂ capture from large point sources.

Communication and dissemination

Conferences participation

First Italian Conference on Carbon Dioxide Capture and Utilisation

December 5-6, 2019. Bari (Italy).

Presentation – CO₂ conversion to light hydrocarbons driven by mechanical activation of olivine powders –
Valeria Farina, from Università degli Studi di Sassari

18° International Congress SAM-CONAMET 2018

October 1-5, 2018. S. C. de Bariloche

CO₂MPRISE Conference results: “Hydrocarbon production from Olivine serpentinisation process” by *Nadia Gamba, Valeria Farina, Gabriele Mulas, Sebastiano Garroni y Fabiana Gennari*

Poster presentations

X Jornadas Chilenas de Catálisis y Adsorción

November 28-30, 2018. Linares, Chile

CO₂ methanation over Ni-Olivine catalysts - *Alessandro Taras, Carlos Navas Cardenas, Adriana Blanco, Sebastiano Garroni, Gabriele Mulas, Francisco Gracia, from Università degli Studi di Sassari*

INCOME2017

September 3-7, 2018. Linares, Chile

Excellence training in solutions for CO₂ capture technology - *Valeria Farina, G. Mulas, S.Garroni, S. Cuesta Lopez, C. Pistidda, I. Yakoumis, N. Vlachos, F.Gennari, F. Gracia, from Università degli Studi di Sassari.*

Other

Seminar- Capture and conversion of CO₂ induced by mechanochemical activation of olivine mineral with water in CO₂ atmosphere

October 21, 2019. Faculty of Sciences of the University of Burgos.

Popularised events

BEERS & BRAINS EVENT

Scientific informal talks addressed to all audiences

October 17th, 2022

Speakers: University of Burgos (Spain) and University of Sassari (Italy)



17 Octubre

BEERS AND BRAINS

Charlas científicas para todos los públicos

Ponentes: Investigadores de la Universidad de Burgos y la Universidad de Sassari (Italia).

 ¿Tienes algo que aportar?

 ¡Estaremos encantados de aprender de ti!

 **18:00 PM**

 **El Carmen 13, Burgos**



UNIVERSIDAD
DE BURGOS



WORLD



BEERS & BRAINS EVENT



Press release 2022

ICCRAM hosts six researchers from international centres and companies

July 28th, 2022

The ICCRAM research centre of the University of Burgos has received six workers from international centres and companies over the last three months, within the framework of the collaboration carried out thanks to the European projects in force. Specifically, they have come from Italy, Greece, Argentina and Thailand, for stays of between one and five months.

*Vassiliki Alexiou, from the Greek company Monolithos, and Fabiana Gennari, from the Centro Atómico Bariloche (CAB-CNEA- Argentina) have joined the team to cooperate in the **CO2MPRISE project**. This project aims to develop innovative materials and processes for CO2 storage and conversion through cross-sectoral synergies between industry and academia.*

For the WORLD project, Matteo Poddighe, from the University of Sassari, and Manfredi Caruso, from the Politecnico di Milano, have come to Burgos. These two Italian collaborators came to support the Burgos company GESTTA, dedicated to the recycling of vegetable oils, in constant contact with ICCRAM. They are working together to develop a recycling and recovery process for used cooking oil.

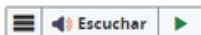
On the other hand, the DRYNET project aims to establish a multidisciplinary network between EU academics, companies and international partners (Japan and Thailand) to share knowledge on dry storage of cells and germplasm. Therefore, Wirakan Kallayanathum and Larindhorn Udomthanaisit have come to UBU from Chulalongkorn University (Bangkok).

Mobility from UBU

This last project has also allowed several ICCRAM researchers to move on a recurrent basis to other associated centres to establish these collaboration and knowledge exchange networks. For example, to companies such as Avantea, in Cremona (Italy), or Biotalentum, in Budapest (Hungary).

Sandra Curiel Alegre (ICCRAM) also spent her pre-doctoral stay from April to June at the Jozef Stefan Institute (Ljubljana, Slovenia) to continue her work on the GREENER project, which combines bioremediation technologies to decontaminate soils contaminated by hydrocarbons. ICCRAM is the international coordinator of this project.





ICCRAM recibe a seis investigadores de centros y empresas internacionales

28
Jul

El centro de investigación **ICCRAM**, de la Universidad de Burgos, ha recibido en los últimos tres meses a seis trabajadores de centros y empresas internacionales, en el marco de la colaboración que se lleva a cabo gracias a los proyectos europeos vigentes. En concreto, han venido desde Italia, Grecia, Argentina y Tailandia, para realizar estancias de entre uno a cinco meses.



Con el objetivo de cooperar en el proyecto CO2Mprise, se han integrado al equipo Vassiliki Alexiou, de la empresa griega Monolithos; y Fabiana Gennari, del Centro Atómico Bariloche (CAB-CNEA- Argentina). Este proyecto tiene el fin de desarrollar materiales y procesos innovadores para el almacenamiento y la conversión del CO2, mediante la sinergia intersectorial entre la industria y el mundo académico.

Para el proyecto WORLD, se han trasladado hasta Burgos Matteo Poddighe, de la Universidad de Sassari, y Manfredi Caruso, del Politécnico de Milán. Estos dos colaboradores italianos llegaron para apoyar a la empresa burgalesa GESTTA, dedicada al reciclaje de aceites vegetales, en constante contacto con ICCRAM. Se trabaja conjuntamente para desarrollar un proceso de reciclaje y valorización de aceite de cocina usado.

Por otro lado, el proyecto DRYNET tiene la finalidad de establecer una red multidisciplinar entre académicos de la UE, empresas y socios internacionales (Japón y Tailandia) para compartir conocimientos sobre el almacenamiento en seco de células y germoplasmas. Por ello, Wirakan Kallayanatham y Larindhorn Udomthanaisit han venido a la UBU desde la Chulalongkorn University (Bangkok).

Movilidad desde la UBU

Este último proyecto también ha permitido que varios investigadores de ICCRAM se trasladen de forma recurrente a otros centros asociados a establecer esas redes de colaboración e intercambio de conocimientos. Por ejemplo, a compañías como Avantea, en Cremona (Italia), o a Biotalentum, en Budapest (Hungría).

Asimismo, **Sandra Curiel Alegre** (ICCRAM), realizó su estancia predoctoral de abril a junio en el Instituto Jozef Stefan (Ljubljana, Eslovenia) para continuar con sus trabajos dentro del proyecto GREENER en el que combina tecnologías de biorremediación para descontaminar suelos contaminados por hidrocarburos. ICCRAM es coordinador internacional de este proyecto.

ICCRAM

International Research Center in Critical Raw Materials for Advanced Industrial Technologies.

El Centro Internacional de Investigación en Materias Primas Críticas para Tecnologías Industriales Avanzadas (ICCRAM) se constituyó en 2014 en la Universidad de Burgos con el objetivo de desarrollar investigación enfocada en las materias primas críticas. Lleva a cabo su actividad en base a proyectos europeos de investigación en tres grupos diferenciados que trabajan bajo sinergias: Grupo ICCRAM Medioambiente, sostenibilidad y toxicología; Grupo de Simulación computacional & Grupo de Procesos electroquímicos y almacenamiento de energía.

DATOS DE LA NOTICIA

Fecha:

Jueves 28 de julio de 2022

Categoría:

PDI

Investigación

INFORMACIÓN Y CONTACTO

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COMPARTIR



Roundtables 2022

Earth day

April 22th, 2022

On the occasion of the Earth Day the CO2MPRISE project organised an online roundtable on new materials and processes for CO2 storage and conversion.

[YouTube Link](#)



Public talks 2022

ICCRAM- Scientific conference series

May 27th, 2022

Sara Rozas (ICCRAM - University of Burgos) gave a talk called "Theoretical approaches on materials design for carbon capture purposes", related to the CO2MPRISE project.

ICCRAM SCIENTIFIC CONFERENCE SERIES
27.05.22





Sara Rozas
Predoctoral researcher at
ICCRAM Materials Design and Modeling group



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ICCRAM- Scientific conference series

July 8th, 2022

Fabiana Gennari, researcher from the Centro Atómico Bariloche (CAB) - CNEA Argentina, gave the talk: "An alliance between hydrogen and carbon dioxide: development of materials for energy decarbonization". This was performed during her 1-month stay at the University of Burgos (Spain).

ICCRAM SCIENTIFIC CONFERENCES
08.07.22



Dra. Fabiana Gennari
Researcher at
CONICET and Centro Atómico Bariloche (CAB) - Instituto Balseiro de Argentina



Knowledge transfer

Computational Methods Course

On 17th – 20th June 2019, the Computational Methods Course for 2D materials was developed for undergraduate and graduate students in the areas related to Chemistry, Physics, Biology or Materials Science. The objective of the training was to give a brief introduction to Quantum Espresso, a useful DFT-based tool for nanoscale calculations and a more detailed view of ORCA, a suitable quantum chemistry program for studying interactions of molecules with 2D materials and their manifestations spectral.

The course was free and open access thanks to the contribution of the European projects H2020 ICARUS, **CO2MPRISE** & SOLUTION and officially recognized by the University of Burgos under the European Transfer Credit System (number of credits to be approved). Two independent sections were addressed:

- A brief introduction to Quantum Espresso, learning how to do some basic calculations using the free Quantum Espresso software. From compilation tips to get a successful set of executables to instructions for drawing useful magnitudes. You also learned how to build input files for different types of calculation. In all cases, the practical sessions will help to fix and practice the concepts acquired during the more theoretical sessions.
- Provide an introduction to Quantum Chemistry using the free ORCA available. Students were able to learn how to obtain structural and electronic information from different systems and how to obtain knowledge about their spectroscopic behavior and their chemical reactivity. Again, the practical sessions were included in the course.

In combination with sessions on computational tools, lectures on 2D materials were delivered by active research in this field. The course also included an attractive social program designed to facilitate interaction between participants on a cultural, scientific and leisure basis.



MOOC: "Developing new technologies in CO2 capture and conversion"

A MOOC on CO2 capture and conversion was recorded in Burgos (Spain), October 2022. Not yet available.

The training is based on **7 modules** and each module has different video chapters.

Module I: CCUS: Carbon capture storage and utilization approach within CO2MPRISE.

Module II: Mechanochemical and Photocatalytic activation of Olivine.

Module III: Innovative Catalytic materials.

Module IV: Metal hydrides.

Module V: MWCN and Graphene for CO2 thermal activation .

Module VI: Synthesis and materials characterisation

Module VII: Conclusions.

Speakers:



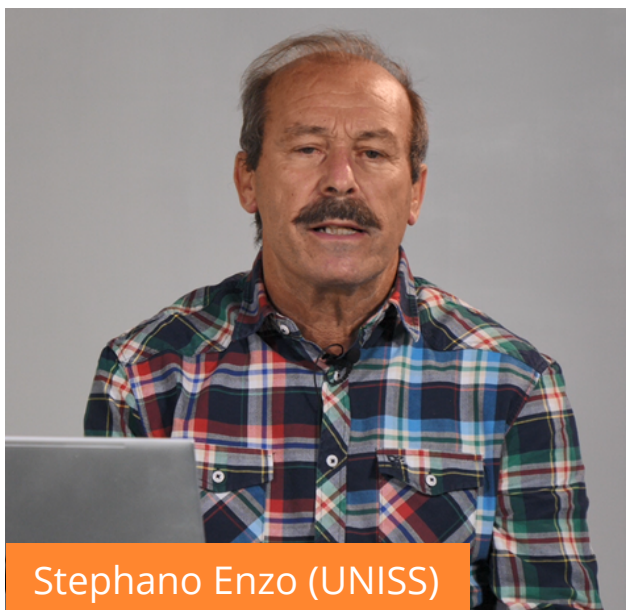
Gabriele Mulas (UNISS)



Fabiana Gennari (CAB, Argentina)



Santiago Aparicio (UBU)



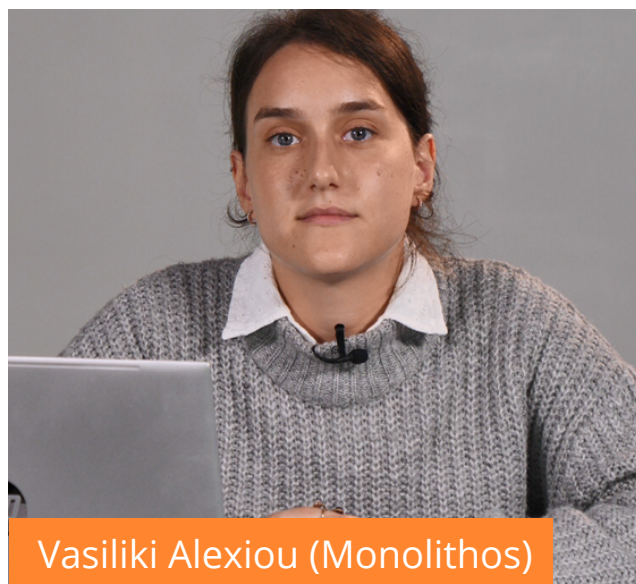
Stephano Enzo (UNISS)



Francisco García (U. Chile)



Carlos Rumbo (UBU)



Vasiliki Alexiou (Monolithos)

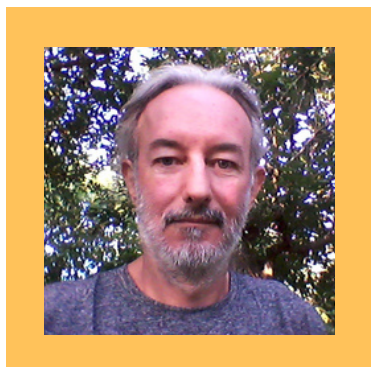


Marios Kourtelesis (Monolithos)



Sebastiano Garroni (UNISS)

Secondees 2022



Pierre Arneodo Larochette

Researcher - Centro Atómico Bariloche (Argentina)

Secondment performed

Università degli Studi di Sassari (UNISS, Italy)

01/07/2022 to 31/07/2022 | 1 month

Objectives

The objectives of his secondment were to learn new experimental techniques and to contribute to the development of materials and methods for the conversion of CO₂ into methane and light hydrocarbons.

Challenges

"There are many challenges, but the most important is being able to incorporate new concepts in a relatively short time".

Activities performed

"We have performed some experiments of CO₂ conversion promoted by ball milling of the material (a mixture of MgH₂, MgO and Ni) under flow conditions".

Lessons learnt

"For me, the greatest learning was related to the coupled use of mechanical grinding and gas chromatography techniques".

Personal experience

"It was a really good experience, from both academic and personal points of view. I meet again with dear friends, Gabriele and Sebastiano, and I was able to work with very kind people like Maria Domenica and Prof. Enzo".



Gabriel Mendoza Santa Cruz - Department of Chemical Engineering, Biotechnology and Materials of the University of Chile

Ph.D. in Sciences of Engineering mention Chemistry and Biotechnology

Secondments performed

- **University of Sassari (UNISS):** 18/05/2022 to 11/08/2022 | 3 months

Objectives

The objectives of his work achieve the synthesis of novel materials based on 2D surfaces metal-oxides as supports for catalyst-support systems applicated in CO₂ reduction to different fuels. In this Ph.D project they aim to synthetize nanolayered materials based on different isolating or semiconducting metal-oxides (zirconia, alumina, ceria, magnesium oxide, among others) for preparing nickel-supported catalysts with enhanced surface area, to test their performance on reducing CO₂ to different fuels under photothermal excitation.

Challenges

One of the main challenges within the project is to obtain the desired nanostructures that can also be a good support and semiconducting system for improving the transformation of CO₂. On the other hand, the construction of a suitable photothermal reactor for the reaction unit is one of the problems that we are currently facing, due its specificity and fine structure.

Activities performed

The main activities have consisted in the characterization and characterization training for X-Ray Diffraction measurements and Rietveld analysis, Scanning electronic microscopy and Transmission electronic microscopy. Furthermore, the team has been collaborating in the design and construction of photo and photothermal reactors for performing the catalytic tests. Finally, one of the activities of this secondment has been the start-up of Quantum Measurement Equipment for measuring photoactive materials and solar cells.

Lessons learnt

"I have learnt several things, particularly in characterization topics, which has been one of my main areas of interests during my degree and Ph.D having the opportunity of learning from the professors, postdoc, students and with the available equipment is a rich experience of learning that can certainly improve the skills of any researcher, besides expanding the number of tools for researching and investigating".

Personal experience

"I had the opportunity to discover a different place with not only a high level in different research fields but also to know a team with a tremendous human quality, which is willing to help everyone who needs it and wants to collaborate and improve their activities by sharing knowledge and ideas. Is very comforting to get to a team of this kind, whose concern of the environmental problem is genuine and involves a multidisciplinary and wide view of science, integrated to different areas and countries that can raise all kinds of solutions".

**Vasiliki Alexiou**

Project manager at Monolithos Catalysts Ltd.

Secondment performed

ICCRAM - University of Burgos (Spain)

01/06/2022 to 31/07/2022 | 2 months

Objectives

The aim of the secondment is to carry out experiments regarding the toxicological evaluation of the catalyst, manufactured by MONOLITHOS.

Activities performed

My main activities, under the guidance of the members of the nanotoxicity lab, are training and experimental work, namely the conduct of toxicity studies applying viability and oxidative stress assays in human cells and the yeast *Saccharomyces cerevisiae* to characterize and clarify the safety of the catalysts.

Challenges and Personal experience

Before my secondment, I had never traveled abroad – so I jumped at the chance. This secondment is a unique experience for me that will definitely help me in the future. I get an invaluable opportunity to travel, train, learn, expand my knowledge and skills and immerse myself in a new culture while making professional connections.

It is also a great opportunity to encourage the exchange of know-how and best practices, with the ultimate goal of finding solutions to reduce CO2 emissions, which is the major challenge of our time.





Fabiana Gennari - Bariloche Atomic Center-National Atomic Energy Commission, National Council for Scientific and Technological Research (CONICET), and National University of Cuyo-Balseiro Institute

Principal Researcher

Secondments performed

- **ICCRAM:** 7/06/2022 to 8/07/2022 | 1 month

Objectives

To develop investigation activities related with CO₂ capture and CO₂ to synthetic fuels conversion processes, mainly using catalysts or hydrides as hydrogen carriers.

Challenges

To identify different reaction mechanisms occurring in presence or in absence of a catalyst, using hydrides and carbonates as hydrogen and carbon dioxide solid sources, respectively. To determine the optimal conditions (temperature, time, H₂:CO₂ ratio) to improve CO₂ conversion to CH₄, reaching high CH₄ yield and selectivity.

Activities performed

I analyzed experimental results obtained during the study of the conversion of CO₂ from mixtures of alkali metal carbonate and alkaline earth metal hydrides. I performed thermodynamic Gibbs free energy minimization calculations to establish the equilibrium compositions as a function of pressure and temperature. Experimental results and thermodynamic predictions were compared to clarify the nature of the reactions involved. I was writing a manuscript to be sent for its evaluation in a top-level international journal on this thematic.

I also participated in a meeting with research groups from the University of Burgos-ICCRAM to analyze experimental results and theoretical calculations, within the framework of the CO₂MPRISE project. New experimental measurements were planned to be performed in Argentina, to complement theoretical calculations carried out by ICCRAM researchers. It was agreed to hold future virtual meetings to advance the development of new CO₂ capture/conversion processes.

In addition, I participated in the following activities:

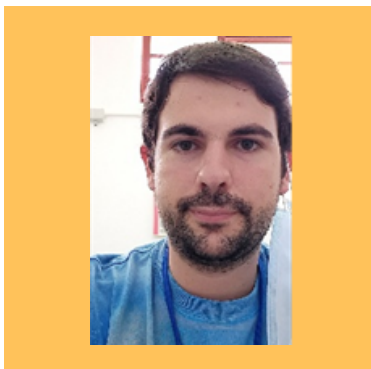
- 1) Two MOOCs were recorded to be released on virtual media about: a) Physico-chemical techniques for investigating CO₂ storage and conversion processes; b) Materials synthesis and processes implementation for CO₂ storage and conversion processes
- 2) A seminar was presented at the University of Burgos-ICCRAM, entitled: An alliance between hydrogen and carbon dioxide: development of materials for energy decarbonization (Friday 8 July, 13:00 h).

Lessons learnt

I emphasize the importance of scientific collaborations.

Personal experience

A fruitful and enjoyable experience. I felt very comfortable in the research group.

**Luca Cappai - UNISS**

Early stage researcher- – PhD Student at University of Sassari

Secondments performed**MONOLITHOS Catalysts Ltd. (Athens, Greece)**

- 21/03/22 to 20/07/22 | 4 months

Objectives

The aim of the secondment was to prepare carbonate based dual phase membranes for CO₂ and O₂ separation from combustion exhaust gases, especially applied to diesel engine heavy-duty vehicles. Permeation test and trials on new carbonates mixtures and ratio to improve membrane activities were performed.

Challenges

Development of carbonate based dual phase membranes supported on stainless steel powder filters have been proposed for CO₂ and O₂ content reduction in exhaust gases. Currently carbonate based membranes work really well only at high temperatures (above 600 °C). In order to be implemented in the target use (diesel engine of heavy-duty vehicles), membranes must reach maximum permeation activity in the range of temperature between 400 °C and 500 °C.

Activities performed

Carbonate based dual phase membranes were prepared by impregnation method. Stainless steel powder filter with 5 µm controlled porosity were used as membrane support. Membranes were prepared with different ratios of alkali carbonate mixtures. Permeation test on prepared membranes were conducted in the range of temperatures 300 °C – 750 °C with GC analysis. XRF measurements were performed on pristine SS powder filters and impregnated membranes before and after permeation tests.

Lessons learnt

Permeation rate is affected not only by carbonate mixture ratio but also by different stainless-steel type supports. Alkali carbonate mixture tested are not suitable to be implemented in HDVs due to their high temperature working range.

Personal experience

My secondment in Monolithos has been a very fruitful and pleasant experience. The exchanges of ideas and discussions were very useful and allowed me to improve my scientific knowledge and methods.



Alessandro Taras - UNISS

Early stage researcher.

PhD Student in the Department of Chemistry and Pharmacy of the University of Sassari.

Secondments performed - UCH Chile

- 17/09/18 to 17/12/18 | 3 months
- 26/03/19 to 26/06/19 | 3 months

Objectives of his work

The work focused on the study of Olivine-based materials doped with nickel, magnetite and cobalt for the conversion of carbon dioxide to methane, following a thermal-promoted methanation process.

Challenges

Development of materials Olivine-based with low environmental impact and low cost, for the conversion of carbon dioxide to fuels such as methane through thermally promoted processes.

Activities performed during his secondments

The experimental activity involved the study of heat-induced conversion processes of carbon dioxide to methane, using Olivine-based systems prepared by ball milling and impregnation as catalysts. The catalysts were subjected to morphological and structural characterization while the reactants and the reaction products in the gaseous state were monitored using a gas chromatograph interfaced with a mass spectrometer.

Lessons learnt

New experimental techniques applied to the transformation of carbon dioxide into products with high added value. Part of the work was presented as a poster at the "X Jornadas Chilenas de Catálisis y Adsorción. 28-30 November 2018, Linares, Chile".

Personal experience

The experience allowed me to create a new working network thanks to which it was possible to expand my scientific knowledge and develop further research tools. Participation in the project allowed me to enrich my personal experience.



Alessandro Taras - UNISS

Early stage researcher.

PhD Student in the Department of Chemistry and Pharmacy of the University of Sassari.

Secondments performed - MONOLITHOS-

- 07/03/22 to 06/08/22 | 5 months
- 22/08/22 to 21/09/22 | 1 month

Objectives of his work

Development of catalysts based on mafic natural silicates and industrial-slag-silicates with low environmental impact and low cost addressed to the conversion of carbon dioxide to fuels through thermally promoted processes. II) CO₂ conversion in liquid fuels (alcohols C1-C4) and/or hydrocarbons using MONOLITHOS Catalysts.

Challenges

CO₂ conversion in liquid fuels (alcohols C1-C4) and/or hydrocarbons using MONOLITHOS Catalysts.

The work focused I) on the study of MONOLITHOS catalysts through the hydrogenation of CO₂; II) on the study of Nickel-based materials supported by Olivine, Basalt, and Steel slag as catalysts for the thermally-activated CO₂ hydrogenation reaction.

Activities performed during his secondments

I) CO₂ hydrogenation with MONOLITHOS catalysts. II) Synthesis, characterization, and study of Ni-Olivine / Basalt / Steel Slag systems as catalysts for the hydrogenation reaction of carbon dioxide thermally induced.

Lessons learnt

Scaling-up of laboratory-scale synthesis for catalyst preparations. Catalysts recycling at the industrial level. During the internship, I attended many seminars and workshops organized by Monolithos.

Personal experience

Participation in the project contributed to broadening my scientific skills, creating a new work network, and enriching my personal experience.

Long term secondees



Sara Rozas Azcona: ICCRAM - Universidad de Burgos

Early stage researcher. Phd student.

Secondments performed

- **Monolithos Ltd.** Spring 2019
- **COMISION NACIONAL DE ENERGIA ATOMICA (CNEA)- Argentina:**

24/09/19 to 23/12/19 | 3 months

13/02/20 to 27/05/20 | 3 months

29/09/21 to 28/12/21 | 3 months

Objectives of her work

During the stays I carried out experimentally the design and characterization of doped solid materials with the aim of improving carbon dioxide affinity with the material, generally metallic ceramics or hydrides.

Challenges

One of the most challenging situation I found was to switch from computers to actual labs. Taking into account the theoretical background behind my previous studies, to deal with reaction times, material weighing or equipment operation, made me derust and develop skills I had left aside.

Activities performed

The feasibility of the reduction of CO₂ to CH₄ employing MgH₂ in the presence and absence of metal catalyst was investigated, exploring different non-independent reaction conditions such as the grade of microstructural refinement, the molar ratio MgH₂:CO₂, reaction time and temperature. Different methanation mechanisms where inferred depending on the reaction conditions. On account of the fact that it was proved that the use of catalyst allows lowering the operational temperature without collapsing the methane yield, this research provides an interesting insight of a thermochemical method for CO₂ reduction to CH₄ employing a solid hydrogen storage medium as H₂ source.

The development of new CexZryO₂-based sorbents have been hindered by a lack of knowledge of the mechanisms ruling CO₂ adsorption on Ce_{0.75}Zr_{0.25}O₂. The structural, electronic, thermodynamic and CO₂ capture properties of monoclinic phases of Ce_{0.75}Zr_{0.25}O₂ were investigated using density functional theory. The results confirmed strong adsorption of CO₂ molecules on all the considered surfaces and materials followed by CO₂ activation as inferred from CO₂ bending, bond elongation and surface to CO₂ charge transfer, indicating CO₂ chemisorption for all cases. Ce_{0.75}Zr_{0.25}O₂ surfaces may be proposed as suitable sorbents for CO₂ capture in wide temperature ranges.

Lessons learnt and personal experience

Experience provided by the stays development have improved my personal abilities regarding laboratory experimental work, feeling comfortable on handling empirical problems. I have also acquired a wide knowledge on synthesis and characterization of target materials, as well as on chemical engineering basics related to carbon dioxide capture and conversion processes. But not only chemistry related skills have been enriched, but communication aptitudes, work-team facilities and personal developing, among others. I would strongly recommend experiencing stays within a European Project.



Alberto Gutiérrez: ICCRAM - Universidad de Burgos

Currently: Margarita Salas postdoctoral researcher at Western Michigan University.

Secondments performed at MONOLITHOS (Athens, Greece)

21/11/17 to 23/12/17 | 1 month

07/01/18 to 08/02/18 | 1 month

07/04/18 to 10/06/18 | 2 months

21/09/19 to 11/12/19 | 3 months

Objectives of his work, challenges and activities performed:

Theoretical molecular simulation studies (molecular dynamics studies, MD, and density functional theory, DFT) in different matrices:

- Complex matrices of porous materials formed by alkali metal carbonates with graphene membranes, carbon nanotubes and fullerenes for efficient CO₂ separation.
- Cerium-zirconium ceramic matrices in contact with copper and palladium-rhodium metal matrices for efficient CO₂ separation and conversion to methane.

In 2019: Theoretical molecular simulation studies (molecular dynamics studies, MD, and density functional theory, DFT) on different matrices, as a continuation of the studies carried out in the previous stays in this company

- Complex matrices of porous materials formed by alkali metal carbonates in stainless steel sheets type 316L for efficient CO₂ capture.

Lessons learnt

To apply for the first time my theoretical knowledge in molecular simulation (DFT and MD studies) to explain and characterize the nanoscopic behavior of different types of materials used in this company for CO₂ capture. Theoretical-experimental approach.

Personal experience

I feel very proud and satisfied with both the work I did in the different secondments and the people I met, which allowed me to develop both personally and professionally outside the scope of my University. This was very good for me, since at that time I was doing my PhD in chemistry.





Alberto Gutiérrez: ICCRAM - Universidad de Burgos

Currently: Margarita Salas postdoctoral researcher at Western Michigan University.

Secondment performed at Centro Atómico Bariloche/Instituto Balseiro (Argentina)

23/09/2018 to 23/12/2018 | 3 months

Objectives of his work, challenges and activities performed:

- Preparation of a mixed lithium-sodium orthosilicate ($\text{Li}_3\text{NaSiO}_4$) by solid-solid reaction.
- Determination of CO_2 adsorption isotherms for such mixed orthosilicate and compare the results obtained with pure Li_4SiO_4 (available measurements).
- Complement the above experiments with XRD and SEM data to see the microstructure of these compounds.
- Finally, start preparing the corresponding theoretical molecular simulation systems (DFT) to complement this experimental study.

Lessons learnt

Learn to use thermogravimetry, XRD and SEM equipment on my own to characterize the lithium and sodium orthosilicates used there for CO_2 capture. Also, to apply my knowledge of molecular simulation (DFT studies) to study the mechanisms governing CO_2 adsorption on lithium orthosilicates (especially $\text{Li}_3\text{NaSiO}_4$) by studying their structural, electronic, thermodynamic and CO_2 capture properties.

Personal experience

I feel very proud and satisfied with both the work I did in the different secondments and the people I met, which allowed me to develop both personally and professionally outside the scope of my University. This was very good for me, since at that time I was doing my PhD in chemistry.



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This project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No 734873

