NEWSLETTER

II 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

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 (SCImago Research Group, Spain 2017).

Website

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) Photoctalytic 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.

Secondees 2022

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

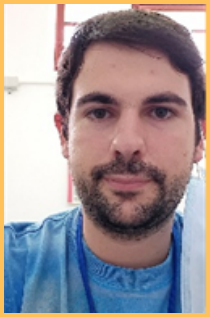
I analyzed experimental results obtained during the study of the conversion of CO2 from mixtures of alkali metal carbonate and alkaline earth metal hydrides. I performed thermodynamic Gibbs free energy minimization calculations to establish the equilibrium compositions as a function of pressure and temperature. 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 Ce0.75Zr0.25O2. The structural, electronic, thermodynamic and CO2 capture properties of monoclinic phases of Ce0.75Zr0.25O2 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. Ce0.75Zr0.25O2 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 (Li_3NaSiO_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 Li_3NaSiO_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.

Other secondees

Nadia Soledad Gamba - CNEA
Experienced Researcher.

PhD in Chemistry at Chemical Engineering Faculty (FIQ) of the National University of Litoral (UNL), Santa Fe, Argentina.

Secondments performed

- **UNISS:** 26/09/17 to 25/11/17 | 19/07/19 to 18/08/19
- **MON:** 19/06/19 to 18/07/19
- **ICCRAM- UBU:** 19/08/19 to 18/10/19

Objectives of her work
Monolithos: study of membranes and reactors for CO2 separation. UNISS: Study of the mineral olivine to capture and convert CO2 to hydrocarbons. Synthesis and characterization. ICCRAM: Synthesis of Mg and Fe silicates and characterization and evaluation of safety cytoxicity effects of the olivine powders.

Challenges
Planning the scientific experiences to optimize the time of my stay. Adapting to unforeseen events and being able to meet the objectives in time. Synthesizing high purity iron and magnesium silicates.

Activities performed during his secondments
Different experimental strategies for the reaction of olivine with CO2 and water by mechanical milling were conducted. Evaluation of membranes for CO2 separation. Discussion of results for the publication of paper (doi:10.3389/fenrg.2019.00107). Characterization of samples before and after CO2 reaction by XRD, SEM and, Raman and FTIR. Experimental in vitro study of toxic effects by direct contact between human cells and olivine after CO2 reaction. Conference for an academic and general audience.

Lessons learnt
Synthetic olivine was successfully synthesized and characterized. Some kind of stress on the cells in contact with olivine after reaction with CO2 was detected. However, then the cells return to base state without effects.

Personal experience
All my secondments have been enriching personal and scientific experiences. I have always been able to work comfortably obtaining high quality results. I have participated in meetings discussing the main results and projecting future research.

Mauricio Damián Arce - CNEA
Experienced Researcher.

PhD in Chemistry at Chemical Engineering Faculty (FIQ) of the National University of Litoral (UNL), Santa Fe, Argentina.

Secondments performed

- **UNISS:** 18/07/19 to 17/08/19

Objectives of his work

The aim of the secondment was to evaluate the interaction of CO2 and water with synthetic magnesium and iron silicates, and the mixture of both (synthetic olivine). This would allow us to understand the role of each constituent of the Olivine mineral in the serpentinization and carbon capture processes.

Challenges

While natural olivine is being under study for its carbon capture capacity, little is known about how each constituent of the mineral affects this process. Being able to individually determine the contribution of each material is highly relevant.

Activities performed during his secondments

Synthesized iron silicate (Fe2SiO4) and commercial magnesium silicate (MgSiO4) were mixed in the proportions naturally found in the olivine mineral. Each silicate and the mixture were analysed during mechanical treatments with water and carbon dioxide at different milling times and at two different rotation frequencies. Gas samples were taken and analysed by Gas Chromatography to quantify the amounts of hydrocarbons, carbon dioxide and hydrogen.

Lessons learnt

Main hydrocarbon product is methane, followed by ethane. CO2 conversion is highly dependent on milling time, evidencing a strong dependence on CO2 sorption for both silicates. Synthetic olivine has worse CO2 conversion with respect to natural olivine.

Personal experience

The secondment at UNISS was a truly fruitful and pleasant experience for his personal and academic formation. The exchange of ideas and discussion of results with colleagues proved to be very enriching for arriving to sounding conclusions.

Valeria Farina - University of Sassari

Early stage researcher.

PhD in Chemical Science and Technology at University of Sassari.

Secondments performed

- CNEA: 19/02/18 to 21/05/18
- MON: 15/11/18 to 17/12/18
- MON: 13/01/19 to 15/03/19

Objectives of her work

Investigation of mechanically induced CO2 storage and conversion driven by olivine weathering process.

Challenges

To study the weathering reaction mechanism of the gas-solid reaction, activated by different type of mill.

Activities performed and lessons learnt

During the first secondment at CNEA in Bariloche she studied the gas-solid reaction between olivine, water and CO2, activated by a planetary mill and I realized the characterization of all the samples through many techniques like XRD, SEM, FT-IR, N2 physisorption, XRF, etc.

During her internship at Monolithos in Athens, she did a literature research related to the study of catalysts used for the conversion of CO2 to Methane.

During the internships, she mostly carried out experimental activities. She attended a conference in Argentina and joined some webinar during her stay in Greece.

Personal experience

The secondments allowed her to increase my scientific knowledge and to establish excellent scientific collaborative relationship.

Carlos Andrés Navas - Universidad de Chile (UCH)
Ph.D. in Chemical Engineering and Biotechnology, University of Chile, 2019.

Secondments performed - UNISS

- 27/02/18 to 28/04/18

Objectives of his work
The main objective of the secondment was to study the effect of Ni promotion for CO2 conversion to Hydrocarbons through the serpentinization reaction. Furthermore, one aim was to perform catalytic tests at different conditions in order to analyze the catalytic activity of Ni-olivine catalysts for the CO2 methanation reaction.

Challenges
To synthesize Ni-olivine catalysts by ball milling process, studying different synthesis conditions and to obtain a high catalytic activity for CO2 conversion to hydrocarbons by mechanochemical and thermal activation at serpentinization conditions.

Activities performed during his secondment
General literature review related to mechanochemical activation and the use of nickel and olivine for CO2 conversion. XRD characterization for Ni-olivine and NiO-olivine samples previously milled from 1 to 40 h. Study of the effect of Ni and NiO concentration on CO2 conversion and its XRD characterization. Effect of the time of pre-ball milling process before the CO2 conversion. Maintenance and calibration of the GC System (Carrier Gas Flow, Column oven temperature and detector calibration).

Lessons learnt
Synthesis of Ni-olivine catalysts by ball milling. Analysis of serpentinization conditions to perform CO2 conversions to Hydrocarbons by mechanochemical activation. Catalyst characterization by XRD, SEM, TEM and BET. Rietvelt Refinement.

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*

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 events

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.

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

Roundtables

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

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.

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 Expresso, learning how to do some basic calculations using the free Quantum Expresso 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.

www.co2mprise.eu

CO2MPRISE PROJECT

CO2MPRISE@UNISS.IT

PROJECT COORDINATOR

GABRIELE MULAS - UNISS
MULAS@UNISS.IT

uniss
UNIVERSITÀ DEGLI STUDI DI SASSARI

UNIVERSIDAD DE CHILE

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