

# **NEWSLETTER**

# 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

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# 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.

## Knowledge transfer

DISSEMINATION EXAMPLE

### **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 <u>Quantum Expresso</u>, 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 <u>Quantum Chemistry</u> 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.



### Some 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.



#### Alessandro Taras - Universidad de Chile (UCH)

Early stage researcher.

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

#### **Secondments performed - UCH**

- 17/09/18 to 17/12/18
- 26/03/19 to 26/06/19

#### 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.



#### 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)

Early stage researcher.

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.

#### **Personal experience**

Professor of Thermodynamics and Transport Phenomena, Vector Calculus and Chemistry. Wastewater treatment and physicochemical characterization. Catalyst synthesis. Materials characterization. Catalytic activity measurements.



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