Annual Report 2020

CO_2PERATE

Cooperation towards a sustainable chemical industry

CO_2PERATE Innovative Training Network
Horizon 2020 research and innovation programme - Marie Skłodowska-Curie grant agreement No. 859910
Contact address: Dept. of Chemistry, UiT The Arctic University of Norway, Tromsø, Norway

Welcome!

CO_2PERATE ITN
Public Annual Report 2020

Table of contents

Overview

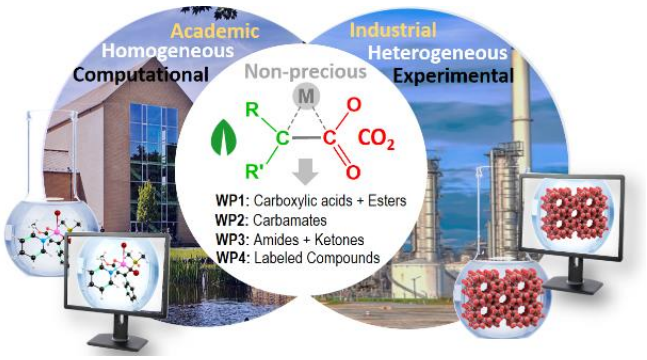
CO_2PERATE: Cooperation towards a Sustainable Chemical Industry

Welcome!

We are proud to present the first Annual Report of CO_2PERATE. By browsing this document, you will learn about CO_2PERATE in several ways: What our research & training goals are, what happened in 2020, some highlights from our research, and finally interviews with our Early Stage Researchers (ESRs).

Who are we?

We are an Innovative Training Network (ITN), funded under the Horizon 2020 research and innovation programme - Marie Skłodowska-Curie grant agreement No. 859910. CO_2PERATE is composed of 10 Beneficiaries (3 industrial & 7 academic) and 2 Partners (see page 4 for all), across 6 European countries. Together we will supervise the training of 15 ESRs towards a PhD degree.



CO_2PERATE has an interdisciplinary and intersectoral research & training program using high level experimental & computational approaches to develop homo- and heterogeneous catalysts for conversion of CO_2 and biomass.

The CO_2PERATE organization is described on page 3 and a double-page feature showing a graphical overview of the whole network on page 18. Our ESRs will tell you more about themselves, their projects and the reasons why they joined CO_2PERATE from page 20.

What is our vision?

The acquisition of new knowledge, the development of new techniques and the training of future chemists is a prerequisite to transform the chemical industry towards a sustainable future. CO_2PERATE has a simple but essential vision: Training of European researchers in the synthesis of indispensable molecules from sustainable carbon sources and with sustainable catalysts. This will involve development of novel and industrially relevant methods for employing CO_2 as a carbon synthon, alongside other renewable biomass, catalyzed by non-precious metals. For highlights of the research ongoing in CO_2PERATE, see page 10, and for a description of ESR projects, see the ESR interviews page 20.

How can you find us?

Email us at co2perate@uit.no, or follow our every day life on social media (Twitter:@co2perate_ITN, FB: @co2perateITN) or on our webpage (co2perate.eu).

Overview

The 10 CO_2PERATE Beneficiaries

UiT The Arctic University of Norway

Catalysis Leibniz-Institut für Katalyse e.V.

Stockholm University

EVONIK POWER TO CREATE

University of Zurich[UZH]

AstraZeneca

UiO : University of Oslo

HALDOR TOPSØE

ICIQ Institute of Chemical Research of Catalonia

AARHUS UNIVERSITY

The 2 CO_2PERATE Partners

RUHR UNIVERSITÄT BOCHUM

RUB

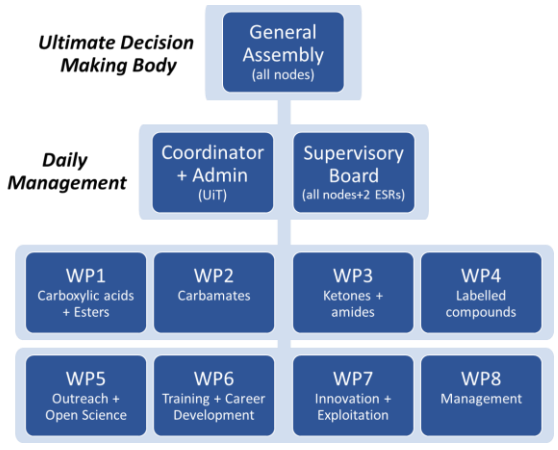
UNIVERSITAT ROVIRA i VIRGILI

Overview

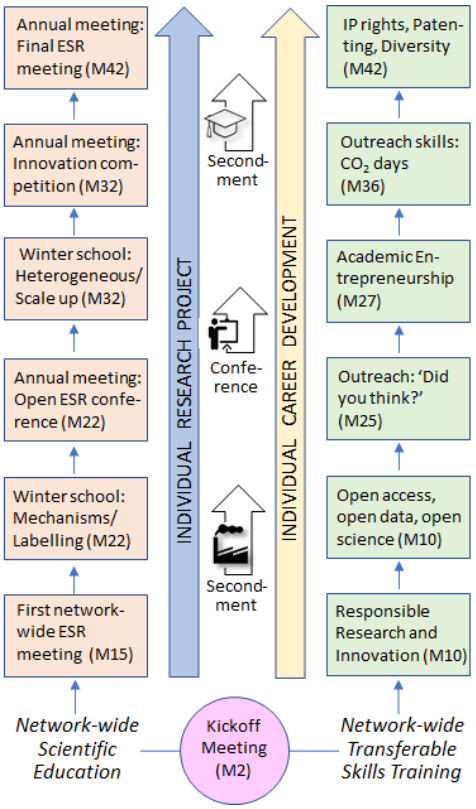
CO_2PERATE Organization

The CO_2PERATE project is funded by the European Commission from 2020 to 2024. CO_2PERATE comprises 10 beneficiaries and 2 partners in 6 European countries. 15 ESRs (PhD students) are planned as part of the action.

The CO_2PERATE research focuses on developing reactions for sustainable conversion of CO_2 to products of higher value. CO_2PERATE has 4 research Work Packages (WPs), which represent the target molecules whose synthesis will involve CO_2: Carboxylic acids & Esters (WP1), Carbamates (WP2), Amides & Ketones (WP3), and Labeled compounds (WP4). 4 additional WPs oversee critical non-research task: WP5 is about Outreach, Dissemination & Open Science, while WP6 tackles Training & Career Development of our ESRs (see figure of training pillars). WP7 focuses on Innovation & Exploitation, and WP8 on Management.



Organization of the CO_2PERATE project.



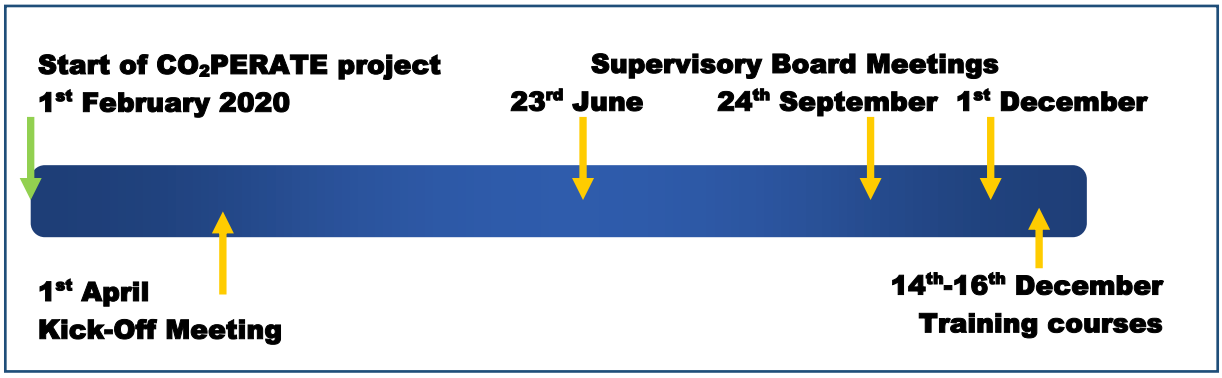
CO_2PERATE training pillars.

The CO_2perate ITN has established a General Assembly (GA), which includes all beneficiaries & partners and is the ultimate decision making body. The daily implementation of the action is ensured by the Supervisory Board (SB), the ITN coordinator (K. H. Hopmann) and the administrative project manager (M.-J. H. Halsør).

CO_2PERATE project leader Kathrin H. Hopmann (left) and dministrative project manager Marie-J. H. Halsør (right, UiT).

Activities

2020 at a glance:

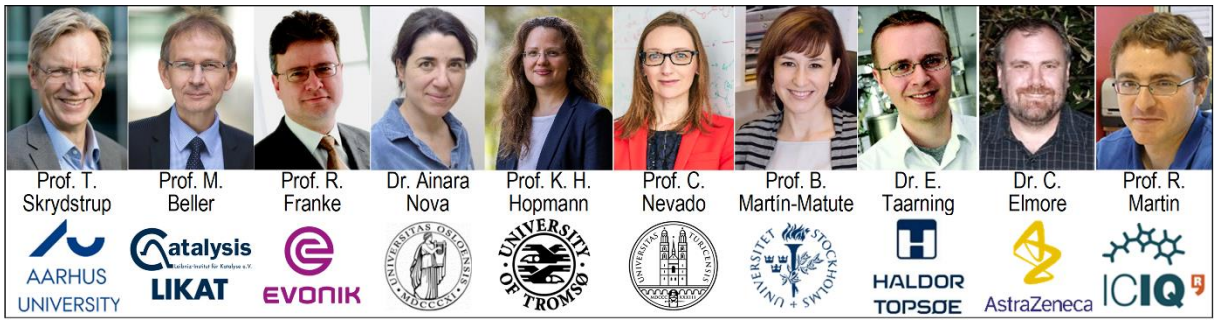


The main focus of CO_2PERATE during 2020 was to recruit 15 early career researchers and to set up the training and research network that should support their scientific growth and career development. Although the activities of CO_2PERATE were influenced by the spreading of the COVID-19 pandemic, with most countries setting up travel restrictions from March 2020, all planned activities were implemented. However, the activities, which originally were meant to take place in Switzerland and Germany, were moved to digital platforms. Read about the details below.

Kick-Off Meeting

1ST APRIL
DIGITAL MEETING

All CO_2PERATE beneficiaries and partners met in a *Zoom* meeting. This included the beneficiaries UiT and UiO in Norway, UZH in Switzerland, ICIQ in Spain, LIKAT and Evonik in Germany, AU in Denmark and SU in Sweden, alongside the partners RUB (Germany) and URV (Spain).



Activities

2020
Supervisory Board Meetings

23RD JUNE
24TH SEPTEMBER
1ST DECEMBER
DIGITAL MEETINGS

The CO_2PERATE Supervisory Board has representatives from all 10 beneficiaries, the 2 partners, alongside two student representatives. The SB has had regular meetings since 2019. In 2020, 3 meetings were held. The recurring themes during these meetings were the recruitment of Early-Stage Researchers (ESRs), the organisation of the ITN courses and, of course, the consequences of the COVID-19 pandemic.

A satisfied, formally established Supervisory Board. Appearing in the picture are the benficiary representatives Esben Taarning (HT), Troels Skrydstrup (AU), Ainara Nova (UiO), Chad Elmore (AZ), Robert Franke (EV), Kathrin Hopmann (UiT), Belen Martin-Matute (SU), SB-substitute Ralf Jackstell (LIKAT) and partner representative Antonio Echavarren (URV), alongside former administrative project manager Trine Andreassen (UIT).


The SB student representatives are Stephanie Ton (AU, left) and Vu Duc Ha Phan (SU, right)

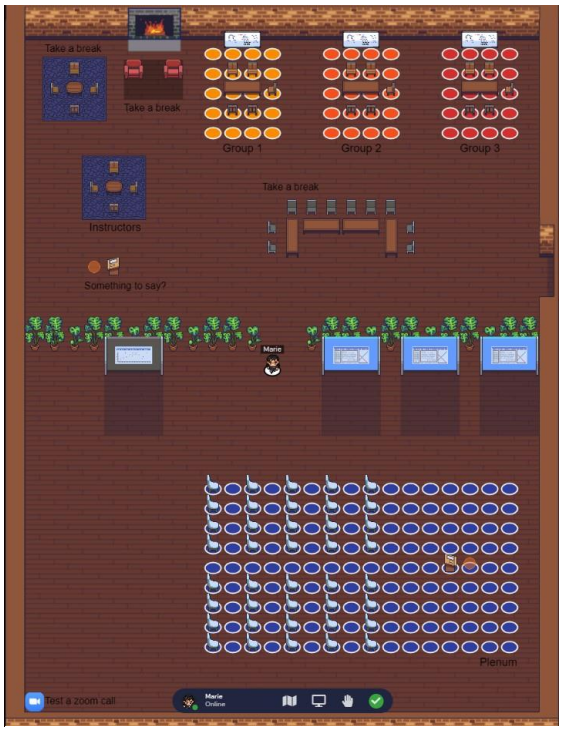
Activities

CO_2PERATE ESR Training Courses

14TH-16TH DECEMBER DIGITAL MEETING

CO_2PERATE organized two ESR training courses in late 2020. The topics for the courses were Open Science (1 day) as well as Responsible Research and Innovation (RRI, 2 days). The courses were planned over 3 days, from 12:00 to 16:00 CET and were hosted by Aarhus University (AU, Denmark), LIKAT (Germany), and UiT (Norway).

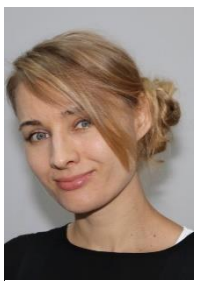
The courses were implemented as external *Zoom* calls within the *Gather*



Map of the location for the 2020 ITN courses, held in Gather.

platform. For this purpose, a map was specially created in Gather.town (see picture) with various areas giving access to the zoom presentations, each day's programme and shared whiteboards for group work, amongst other features. Each course day consisted of several lectures by invited speakers and a group work session followed by a general discussion in plenum.

The first day, hosted by AU, offered our ESRs the opportunity to learn about open access publishing, deposition of research data online and open science collaborations between academia and the industry. The lectures of the day were given by Marie-Louise Conradsen, Head of Open Science at the Faculty of Natural and Technical Sciences at Aarhus University (AU) and Morten Hjorth Gad, Librarian at the Royal Danish Library in Aarhus. The chosen topic for the lectures were Open Science and Open Access, respectively.

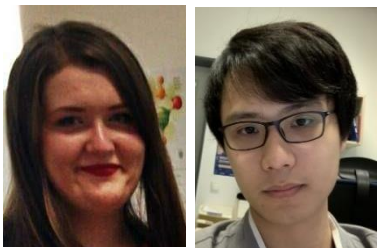


Invited speakers Marie-Louise Conradsen and Morten Hjorth Gad gave talks on the first day of the course.

Activities

The group work session focused on Data Management, the FAIR principles and open access publishing models. The ESRs were also reflecting upon the concepts of Open Data and Open Science.

Both the second and third course days dealt with RRI, each day on a different sub-topic. LIKAT hosted the first part, focused on Best practices and Scientific Misconduct. Insights on what constitutes unacceptable behaviour in a research environment were provided during the lecture by Prof. Matthias Beller (LIKAT), while LIKAT ESRs Martina Perlog and Weiheng Huang familiarized the audience with the European Code of Conduct for Research Integrity and the United Nations Sustainability Goals, respectively. The former was also the chosen topic of the group work session,



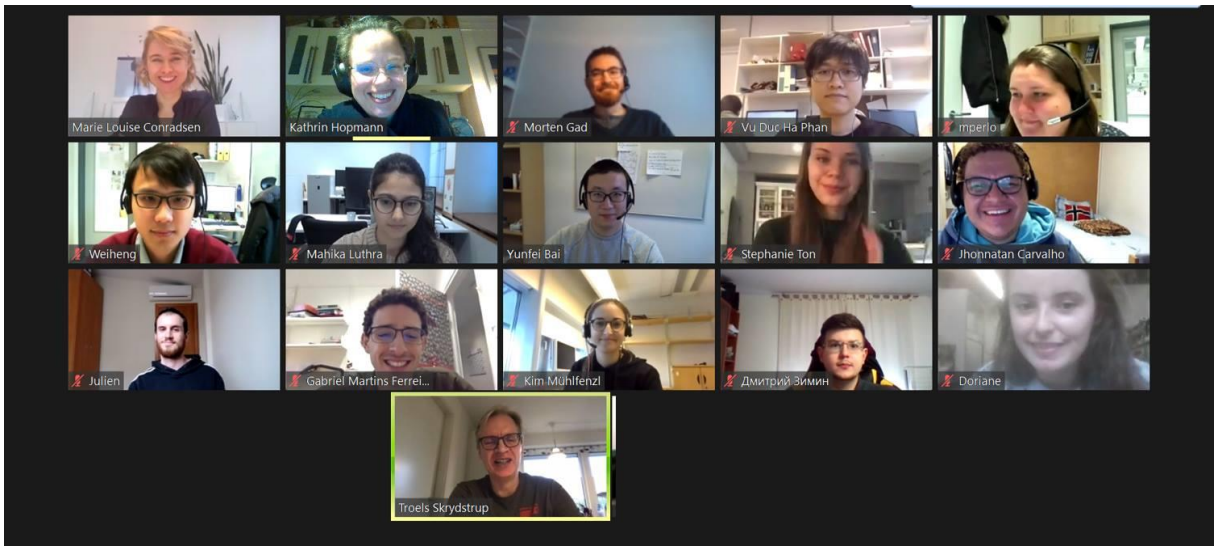
The team from LIKAT, with ESRs Martina and Weiheng and their supervisor Matthias Beller, organized the first RRI session day.

Invited speakers Jessica Wade and Sophie Janbon provided insights on diversity within both academia and the industry.

with questions about the four principles of Reliability, Honesty, Respect and Accountability. The ESRs were given the opportunity to reflect on plagiarism, data fabrication and the meaning of author contributions to a research publication.

The final day of the course, hosted by UiT, concentrated on the topics of diversity and outreach. The topic of diversity was explored by invited speakers Dr. Jessica Wade from the Imperial College of London and Dr. Sophie Janbon (AZ), giving perspectives from both academia and industry. During the group work session, ESRs had the opportunity to map the diversity within their groups as well as reflect on including (and excluding) behaviours. They also pondered whether diversity and gender balance are the same thing. The topic of outreach was also treated during the group work sessions, focusing on the researcher's responsibility to reach out to society.

Activities



The CO_2PERATE PhD students at the RRI course. Also in the picture CO_2PERATE PIs Kathrin Hopmann (UIT) and Troels Skrydstrup (AU) and the Open Science presenters Marie Louise Conrad (AU) and Morten Hjorth Gad (AU).

What's next in CO_2PERATE?

The pandemic might still be raging but we have a lot planned for 2021 – for now digitally. The biggest event of the year will be the Mid-term Check Meeting with our Project Officer from the Research Executive Agency, which will take place at the end of April 2021. We will use this occasion to hold separate activities for our ESRs on the theme of career development.

2021 will also see the organisation of recurring events for the sole purpose of keeping in touch. Indeed, networking through idle talk - usually done in between sessions at a conference - has been something missing from our (digital) lives. The meetings, held every first Wednesday of the month, are the occasion to meet in a more informal way and thus actually get to know each other outside of structured activities.

We are also looking forward to organising our 2021 Annual Meeting and Winter school. Whether those will be held as physical meetings remains to be seen.

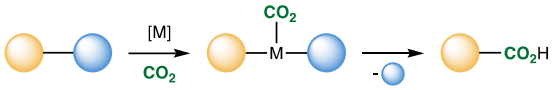
Last but not least the Supervisory Board continues to meet regularly.

Research

A closer look at...

PROJECT 1
ICIQ
DMITRY ZIMIN

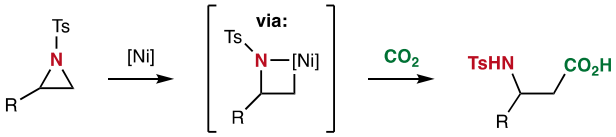
Project 1 “Catalytic carboxylation of saturated hydrocarbons with CO_2 en route to fatty acids” is part of Work Package 1 (WP1, “Carboxylic Acids and esters from CO_2”). The project is hosted by ICIQ under the supervision of Prof. Rubén Martín and its goal is the development of novel and efficient metal-catalyzed carboxylation reactions of different organic matters. Indeed, the utilization of CO_2 as a carbon source in organic synthesis to obtain carboxylic acids and their derivatives is under intense scrutiny of the community.[1]



General concept of metal-catalyzed carboxylation reactions

Recently, in Martín’s group, we found that such important synthetic building blocks as beta-amino acids can be obtained by carboxylation of aziridines in a catalytic manner in the presence of nickel complexes. Potentially, the reaction proceeds through the formation of azanickella-cyclobutanes, which can react with CO_2 to achieve the desired product.[2,3]

Some advantages of the developed methodology are mild reaction conditions, a high functional group tolerance, and the availability of starting aziridines from simple olefin feedstocks or amino alcohols. Moreover, the present reaction can be implemented for the synthesis of pharmaceutically relevant products as well as ^{13}C labeled beta-amino acids. The corresponding manuscript was recently accepted for publication in the JACS and we expect the results to be accessible soon.



Nickel-catalyzed carboxylation of aziridines.

References:

1. Tortajada, A.; Juliá-Hernández, F.; Börjesson, M.; Moragas, T.; Martin, R. Transition-Metal-Catalyzed Carboxylation Reactions with Carbon Dioxide. Angew. Chemie Int. Ed. 2018, 57 (49), 15948–15982.DOI: 10.1002/anie.201803186.

2. Lin, B. L.; Clough, C. R.; Hillhouse, G. L. Interactions of Aziridines with Nickel Complexes: Oxidative-Addition and Reductive-Elimination Reactions That Break and Make C-N Bonds. J. Am. Chem. Soc. 2002, 124 (12), 2890–2891. DOI: 10.1021/ja017652n.

3. Somerville, R. J.; Odena, C.; Obst, M. F.; Hazari, N.; Hopmann, K. H.; Martin, R. Ni(I)–Alkyl Complexes Bearing Phenanthroline Ligands: Experimental Evidence for CO 2 Insertion at Ni(I) Centers. J. Am. Chem. Soc. 2020, 142 (25), 10936–10941. DOI: 10.1021/jacs.0c04695.

Research

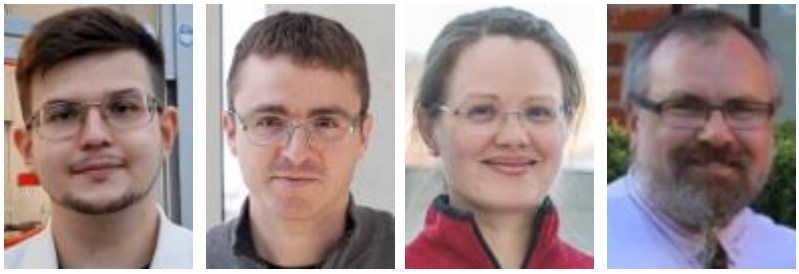


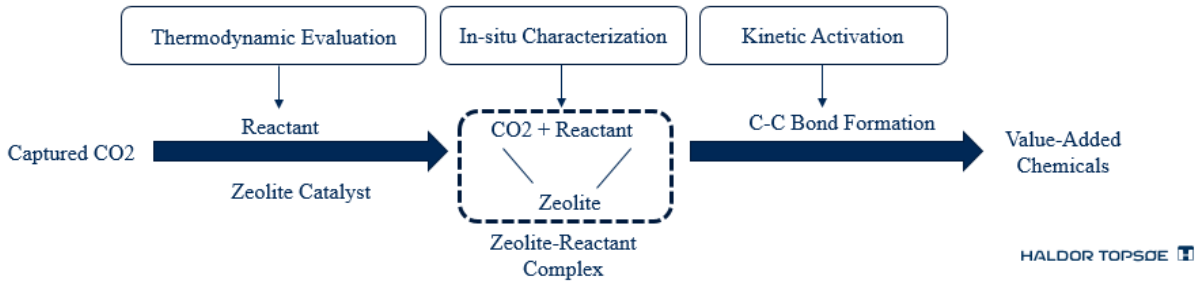
Figure 1. Early-stage researcher Dmitry Zimin with his main supervisor Rubén Martín (ICIQ), and the co-supervisors Kathrin H. Hopmann (UiT) and Chad Elmore (AZ).

A closer look at...

PROJECT 4
HALDOR TOPSØE
YUNFEI BAI

With the rapid development of modern industries, emissions of CO_2 have been one of the main contributors to the climate crisis that threatens to increase global temperatures. New technologies to capture and utilize CO_2, reintroducing it as a carbon-based feedstock for producing chemical products, would be an ideal way to mitigate new emissions and at the same time create value.[1]

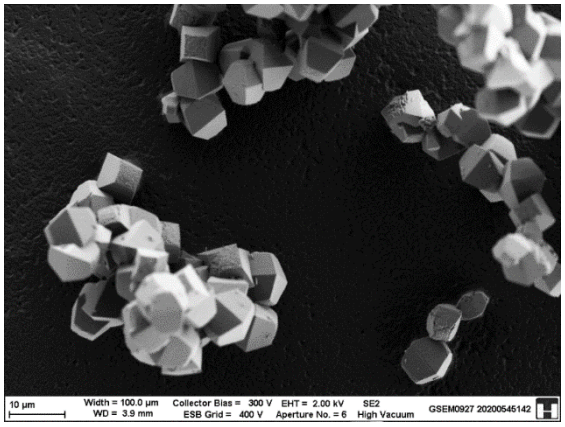
Project 4 is entitled "C–C bond forming reactions with CO_2 using Lewis acidic zeolite catalysts" and is part of Work Package 1 (WP1, "Carboxylic acids and esters from CO_2"). Zeolites are solid acid catalysts with very large surface areas that provide them with high active sites densities. Some of their industrial application as catalysts are into hydrocracking of oil derivatives, isomerization and alkylation in petrochemicals or gasoline/olefins production from methanol.[2] Recently, Lewis acid zeolites have been found to be effective to activate C=O bond in reactions involving sugar conversion, making these materials interesting as potential catalysts to activate a similar type of bond in the CO_2 molecule.[3]



A schematic overview of project 4 (figure: Haldor Topsøe).

Research

In this project, we aim to explore the use of CO_2 as raw material for value-added chemicals. Initially, thermodynamic feasibility of a wide range of reactions involving CO_2 and other reactants in C-C coupling, is being theoretically evaluated.



Scanning electron microscope (SEM) image of a zeolite catalyst (picture: Haldor Topsøe).

After the identification of the most thermodynamically favored reactions, the interaction of CO_2 and other reactants with zeolitic catalysts will be investigated using advanced characterization techniques. Subsequently, the kinetic activation of CO_2 will be experimentally evaluated over selected catalysts, in a step that will optimize reaction conditions considering thermodynamics and reactants-catalyst interactions. Apart from creating a process that could potentially lead to an effective utilization and valorization of CO_2, we also aim to acquire important knowledge on the challenging CO_2 activation topic and share these findings within our ITN network to push forward CO_2PERATE project together.

References:

1. Maginn, E. J. What to Do with CO_2. *The Journal of Physical Chemistry Letters* **2010**, 1, 3478-3479. DOI: 10.1021/jz101582c

2. Corma, A. State of the Art and Future Challenges of Zeolites as Catalysts. *Journal of Catalysis* **2003**, 216, 298-312. DOI: 10.1016/S0021-9517(02)00132-X

3. Holm, M. S.; Saravanamurugan, S.; Taarning, E. Conversion of Sugars to Lactic Acid Derivatives Using Heterogeneous Zeotype Catalysts. *Science* **2010**, 328, 602-605. DOI: 10.1126/science.1183990

Early-stage Researcher Yunfei Bai with his main supervisor Esben Taarning (HT), and his co-supervisors Ainara Nova (UiO) and Troels Skrydstrup (AU).

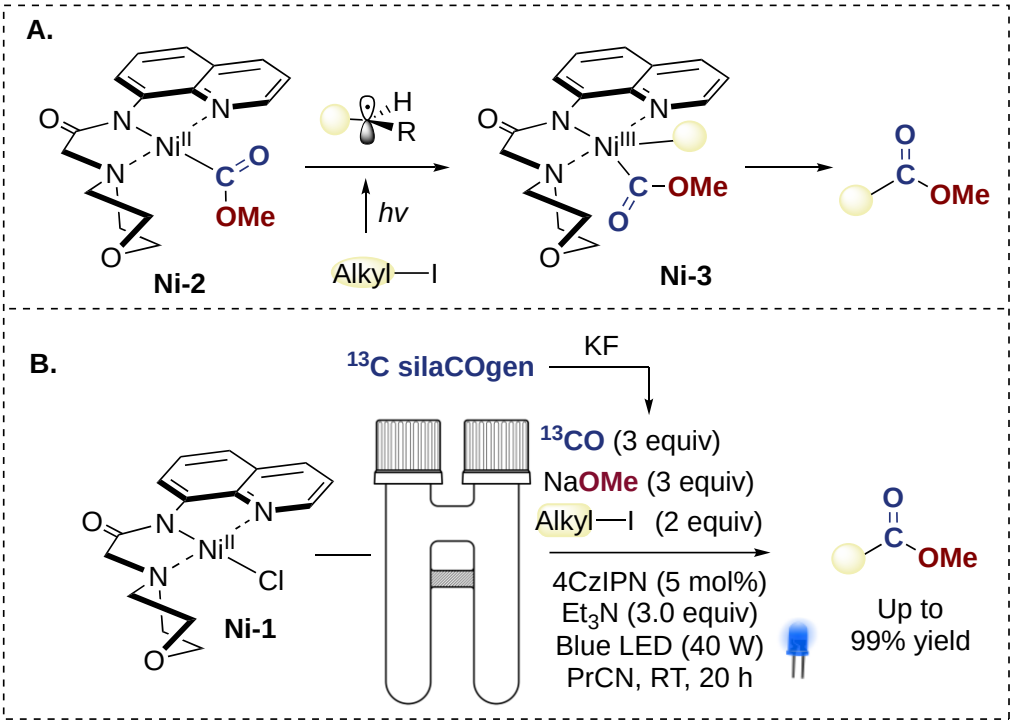
Research

A closer look at...

PROJECT 9
AARHUS UNIVERSITY
STEPHANIE TON

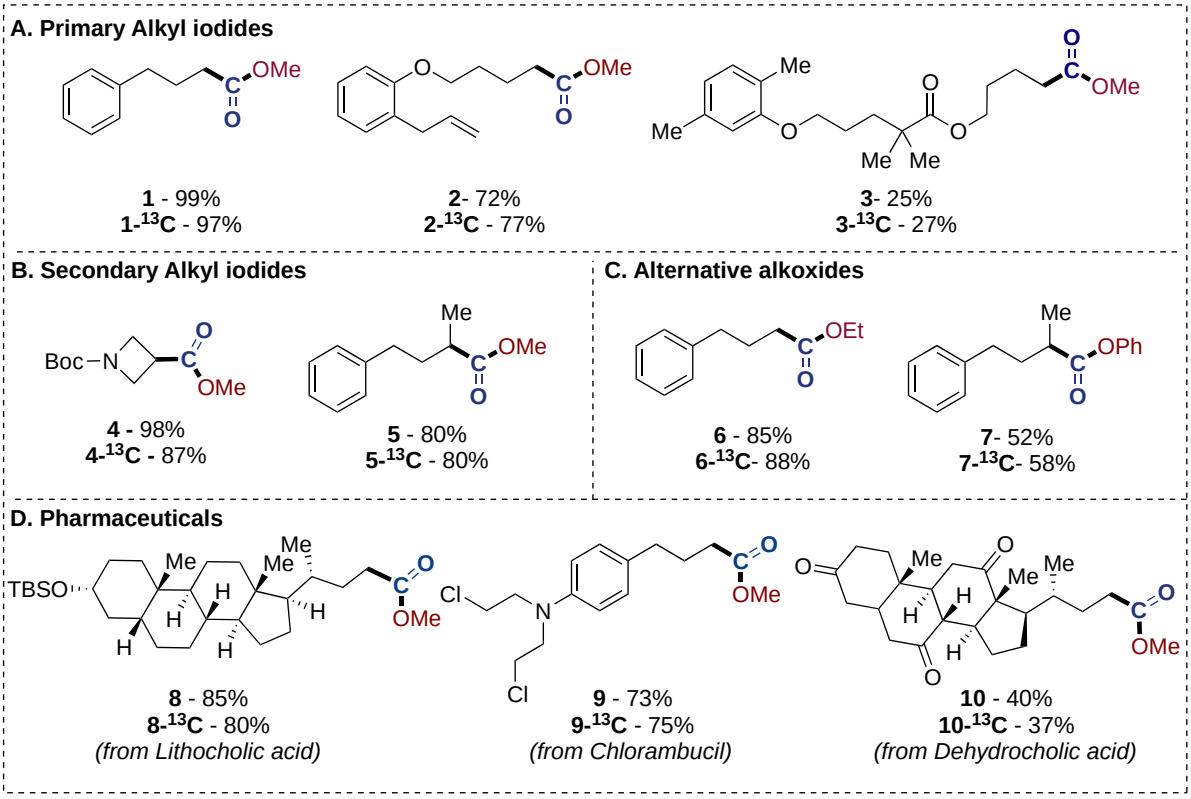
Project 9 is titled “Efficient Methods for CO_2 Conversion to CO and PET labelling of pharmaceuticals” and is a part of both WP3 (“Amides and ketones from CO_2”) and WP4 (“Labelled compounds from CO_2”). The goal of this project is to streamline the efficient and late-stage incorporation of carbon isotopes into bioactive molecules. For this purpose, we sought to prepare labelled esters via a nickel mediated carbonylative coupling approach, for this we utilized nickel pincer complex **Ni-1** as it is well documented to undergo CO insertion from Ni-Alkyl species.[1] Initial reaction with sodium methoxide followed by ^{13}CO insertion would give a nickel species bearing a labelled carboxylate functional group **Ni-2**. Addition of an open-shell radical and subsequent reductive elimination would then deliver the targeted C-C linkage in fully labelled methyl ester derived from the alkyl halide.[2]

Reaction conditions for this transformation were developed, utilizing 2-chamber glassware for the ex-situ generation of stoichiometric ^{13}C-labelled carbon monoxide from crystalline precursor silaCOgen.[3] The photochemical activation of the alkyl



Preparation of labelled esters using a nickel-mediated carbonylative coupling approach. Panel A: initial hypothesis for nickel carboxylate utilisation. Panel B: optimized reaction conditions for methyl ester formation. (Figure: S. Ton)

Research



Partial scope of Ni-mediated synthesis of aliphatic esters with and without ^{13}C. (Figure: S. Ton)

iodides is carried out via halide atom transfer upon treatment of the alkyl iodide with the organic photocatalyst 4CzIPN, triethylamine, and blue LED irradiation.[4] In the screening of reaction conditions, it was found that an excess of the alkoxide (NaOMe, 3 equivalents) and an increased pressure of carbon monoxide (3 equivalents) in the solvent butyryl nitrile led to optimized yields (99% yield **1**).

From these optimized conditions, a scope of labelled esters was prepared from alkyl iodides. With standard reaction conditions, methyl esters were obtained in good yields from a variety of primary alkyl iodides. The conditions were found to tolerate a variety of functional groups including aryl/alkyl halides and olefins, as well as compound **8,** which contains an ester functionality and was prepared in moderate yields. For secondary alkyl iodides, LiOMe was utilized in place of sodium methoxide and the reaction time was increased from 20 to 48 hours. This change greatly reduced the amount of side product formation derived from the base-induced elimination of the alkyl iodide.

Utilization of other alkoxide nucleophiles was also possible and ethoxy- and phenoxy- esters were obtained in good yields. Sodium phenoxide primary alkyl iodides were not utilized due to competing substitution reactions. Finally, pharmaceutical derivatives were prepared from their commercially available carboxylic acids via a procedure described by Fu *et al.*[5] The carboxylic acids were first converted to

N-(acyloxy)phthalimide, subsequent triphenylphosphine-catalysed alkylative iododecarboxylation with lithium iodide under blue LEDs gave the desired alkyl iodide. Subjecting the alkyl-iodides to the standard reaction conditions gave the isotopically labelled pharmaceutical derivatives of lithocholic acid, chlorambucil and dehydrocholic acid in good yields with 100% isotope incorporation.

This work lays out a preparative methodology for the late-stage incorporation of labelled carboxylate functionalities via a nickel-mediated carbonylation reaction. This methodology was utilized for the synthesis of methyl esters from both primary and secondary alkyl iodides in addition methyl ester derivatives of pharmaceutical compounds were prepared in good yields. The reaction was initially perceived to proceed by the initial formation of a Ni(II) carboxylate structure (**Ni-3**) however, subsequent stoichiometric experiments suggest that alternative pathways are operative and further mechanistic studies are currently underway. Finally, this methodology highlights new reactivity for the pincer complex **Ni-1** and offers new insights in future endeavours to develop labelled pharmaceuticals.

References:

1. Neumann, K. T.; Donslund, A. S.; Andersen, T. L.; Nielsen, D. U.; Skrydstrup, T., Synthesis of Aliphatic Carboxamides Mediated by Nickel NN2-Pincer Complexes and Adaptation to Carbon-Isotope Labeling. *Chemistry - A European Journal* **2018,** *24*, 14946-49. DOI: 10.1002/chem.201804077

2. Donslund, A. S.; Pedersen, S. S.; Gaardbo, C.; Neumann, K. T.; Kingston, L.; Elmore, C. S.; Skrydstrup, T., Direct Access to Isotopically Labeled Aliphatic Ketones Mediated by Nickel(I) Activation. *Angewandte Chemie International Edition* **2020,** *59*, 8099-8103. DOI: 10.1002/anie.201916391

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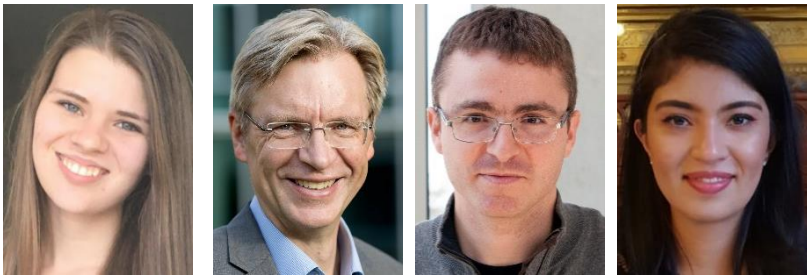
5. Fu, M.-C.; Wang, J.-X.; Shang, R., Triphenylphosphine-Catalyzed Alkylative Iododecarboxylation with Lithium Iodide under Visible Light. *Organic Letters* **2020,** *22*, 8572-77. DOI: 10.1021/acs.orglett.0c03173

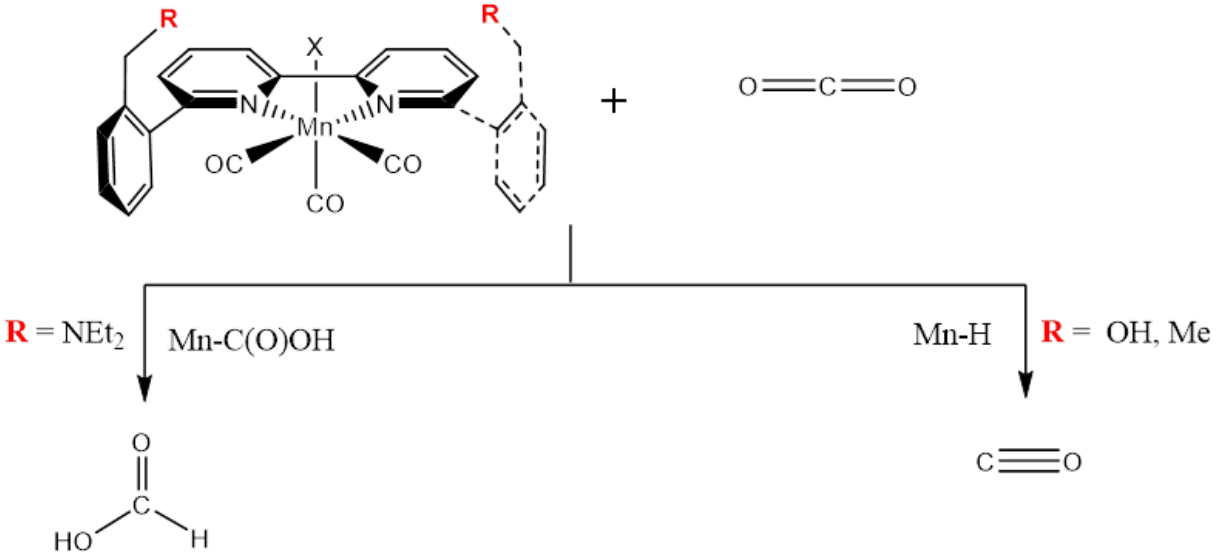


Early-stage Researcher Stephanie Ton and her main supervisor Troels Skrydstrup (AU), and co-supervisors Rubén Martín (ICIQ) and Malvika Sardana (AZ).

Research

A closer look at...

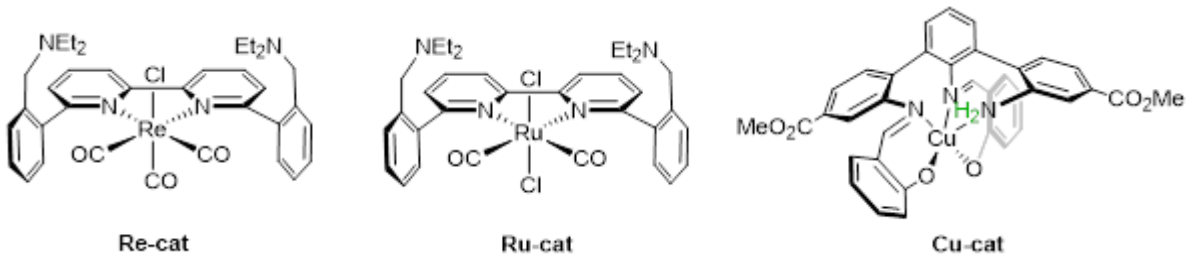
PROJECT 10
UNIVERSITY OF OSLO
MAHIKA LUTHRA



Reaction scheme for the reduction of CO_2 in the presence of amines. (Figure: Rønne, M. H et al.[1])

Project 10, entitled "Computational insights into the conversion of CO_2 to CO and carbonylation reactions", is a part of WP3 ("Amides and ketones from CO_2"). Its goal is to establish mechanisms for the reduction of CO_2 and carbonylation reactions using MOF-supported catalysts.

Controlling the selectivity for different CO_2 reduction products is a major challenge for experimentalists. The group of CO_2PERATE PI Troels Skrydstrup[1] (AU) has reported a series of manganese carbonyl complexes with elaborated bipyridine or phenanthroline ligands that can reduce CO_2 to either formic acid if the ligand structure contains strategically positioned tertiary amines; or to CO if amine groups are absent from the ligand.



Some of the amine complexes used in this study. (Figure: Rønne, M. H et al.[1])

Research

I have started computing the mechanism for the electrochemical reduction of CO_2 with similar systems containing different metal centres such as **Re-cat** and **Ru-cat**[2-3]. I am also studying the role of amines in other systems like that of **Cu-cat**, which was synthesized by the catalysis group at UiO. The calculations are carried out using the Gaussian program. Currently, I am using the Re system to determine which are the best functionals and basis sets to describe this system.

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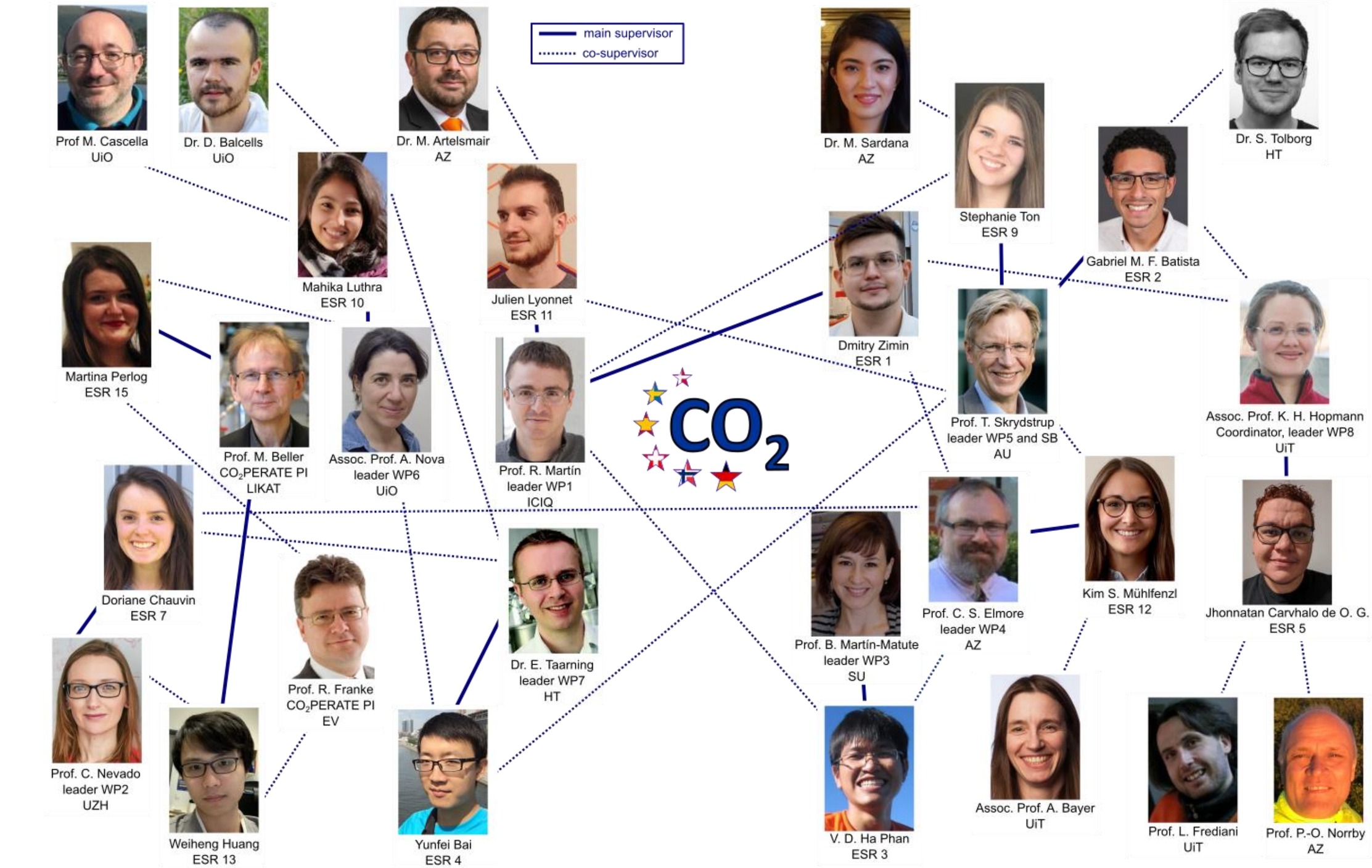
2. Bhattacharya, M., Sebghati, S., VanderLinden, R. T., & Saouma, C. T. (2020). Toward Combined Carbon Capture and Recycling: Addition of an Amine Alters Product Selectivity from CO to Formic Acid in Manganese Catalyzed Reduction of CO 2 . *Journal of the American Chemical Society*, *142*, 17589–17597. DOI: 10.1021/jacs.0c07763
3. Madsen, M. R., Jakobsen, J. B., Rønne, M. H., Liang, H., Hammershøj, H. C. D., Nørby, P., Pedersen, S. U., Skrydstrup, T., & Daasbjerg, K. (2020). Evaluation of the Electrocatalytic Reduction of Carbon Dioxide using Rhenium and Ruthenium Bipyridine Catalysts Bearing Pendant Amines in the Secondary Coordination Sphere. *Organometallics*, *39*, 1480–1490. DOI: 10.1021/acs.organomet.9b00815

Early-stage Researcher Mahika Lutra, her main supervisor Ainara Nova (UiO), and her co-supervisors Esben Taarning (HT), David Balcells (UiO) and Michele Cascella (UiO).

The CO_2PERATE Innovative Training Network



Early-stage Researchers

Dmitry Zimin

ESR #1
ICIQ

Dmitry obtained his Masters degree from the Saint Petersburg State University, Russia. In his free time, he enjoys swimming and reading both popular science and literature classics.

Why did you join CO_2PERATE?

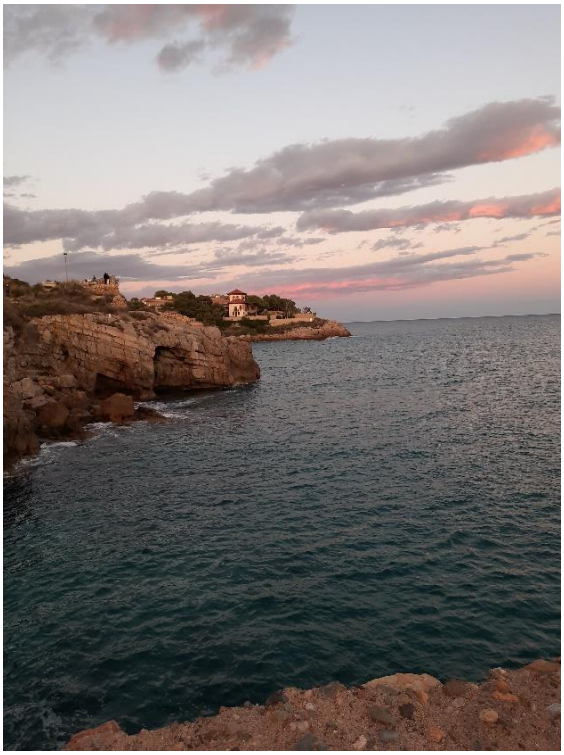
I joined CO_2PERATE because this PhD program combines modern organometallic chemistry (which is my favourite field of chemistry) and the actual problem of carbon dioxide excess in our environment. It gives me the feeling of high responsibility which I found inspiring, and inspiration is a main engine of science.

What is your project about?

In my project, I investigate possibilities to obtain chemical reactivities between carbon dioxide and different organic matters. It requires specific "cocktails" of reagents, and in the case of my project, the cornerstone is a transition metal that acts as a bridge, which allows carbon dioxide and the organic compound to react with each other. Products of such interactions are normally carboxylic acids, an important class of compounds widely used in different areas of the chemical industry. Recently, we found a way to obtain beta-amino acids, using carbon dioxide fixation and I hope we will soon present to the society the results of our investigations.

Tell us about the institution/country you are currently in.

I do my research project at the Institute for of Chemical Research of Catalonia (ICIQ) under the supervision of Prof. Ruben Martin. ICIQ is one of the most competitive research institutes in the world and provides for research all



A beautiful view on the Balearic seaside in the evening, Tarragona, Spain. (Photo: D. Zminin)

state-of-the-art facilities for modern science. Additionally, a broad network of contacts allows young scientists to have collaborations with colleagues from all around the world. Finally, ICIQ is located in Catalonia, which is one of the most beautiful places in the world. Altogether, these factors make ICIQ an ideal place for studies and research.

Is there one thing about you that you would like others to know?

I am in love with Spanish tortillas.

Platja del Miracle, Tarragona, Spain. (Photo: D. Zminin)

Dmitry's main supervisor Rubén Martín (ICIQ), and co-supervisor Kathrin H. Hopmann (UiT) and Chad Elmore (AZ).

Gabriel Martins Ferreira Batista

ESR #2
AU

Gabriel obtained his Master's Degree from the Federal University of Juiz de Fora, Brazil. He enjoys spending his free time with friends and family.

Why did you join CO_2PERATE?

While searching for a Ph.D. position, I was aiming at something that could unite my interest in organic synthesis and in catalysis. Within this topic, the valorisation of lignin through carbonylation stood out. Furthermore, I saw that the CO_2PERATE ITN could give me the opportunity to work in collaboration with diverse experts in different fields of chemistry.

Early-stage Researchers

What is your project about?

My project involves the catalytic conversion of lignin models to aryl carboxylic acids. The purpose is to valorise lignin which is mainly a waste product from the paper industry.

Tell us about the institution/country you are currently in.

I am doing my Ph.D. at AU, Denmark. So far, I like both the university and the country a lot. The people are friendly and try to help you whenever they can.

Gabriel's main supervisor Troels Skrydstrup (AU), and co-supervisors Kathrin H. Hopmann (UiT) and Søren Tolborg (HT).

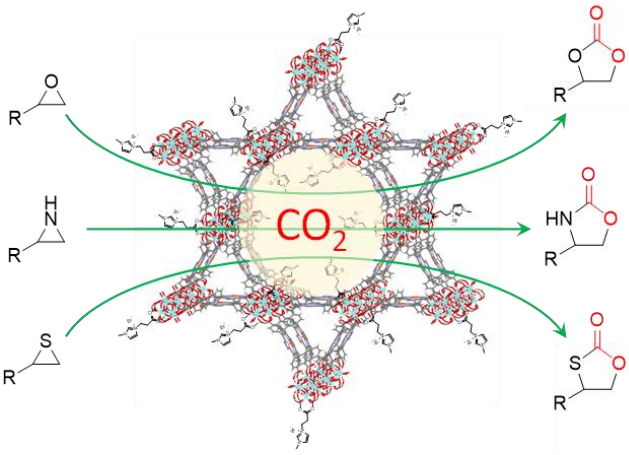
Vu Duc Ha Phan

ESR #3
SU

Ha obtained his Master's Degree from the National Tsing Hua University in Taiwan and has worked 3 years as a R&D researcher for Hyosung Vietnam. In his free time, he enjoys mountaineering and trekking.

Why did you join CO_2PERATE?

My entire study and work period is to deal with practical problems in industry and to bring the academic concepts to life. I finished both of my Bachelor's and Master's degree in the field of Chemical Engineering and later became a manager in Department of Research and Development of an industrial company.

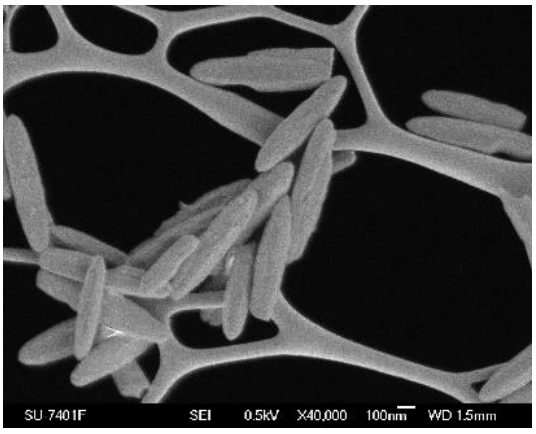


Ha's project takles the challenge of designing cycloaddition reactions at room temperature, without nuclephilic additive, that have a high turnover frequency and employ reusable catalysts. (Figure: V. D. H. Phan)

Early-stage Researchers

Those are precious experiences and have assisted me very well in my career.

Being a PhD student in Organic Chemistry at Stockholm University and an ESR in CO_2PERATE project has been a milestone of my life. I have been offered numerous opportunities to meet other ESRs and experts around the world whom I can learn from. Besides, CO_2PERATE with its industrial collaboration is definitely a great environment where my knowledge and expertise can thrive.



Scanning Electron Microscopy (SEM) image of Ha's Hafnium-based heterogeneous catalyst (Image: V. D. H. Phan)

What is your project about?

My current project is to develop a series of heterogeneous catalysts which can be used for chemical transformation reactions such as cycloaddition reaction using CO_2. Utilizing CO_2 as a building unit of chemical substances can reduce the dependence on fossil fuel in chemical industry. The catalysts can be effectively reused several times, so it is promising for a low-cost eco-friendly method of producing chemical compounds.

Tell us about your institution/country you are currently in.

Stockholm University is located to the north of the Stockholm city centre and is surrounded by national city parks. Getting out into nature is never that easy if you are a student at SU.

"*Not too little. Not too much. Just right!*"

That quote or Lagom is the secret of living a balanced, happy life of Swedish people. You can always find a little happiness, a favourite place that suits you the most when you are here, Sweden.

The Frescati campus (left) at Stockholm university and the Riddar Island in the Gamla Stan area of Stockholm, Sweden. (Photos: Clément Morin for Stockholm University and Mikael Damkier)

Early-stage Researchers

Is there one thing about you that you would like others to know?

In case people are interested. I'm in love with this dish so-called "bánh xèo". It is a Vietnamese traditional pancake, the name literally translates to "sizzling cake", after the sound the rice batter makes when it is poured into the hot pan.

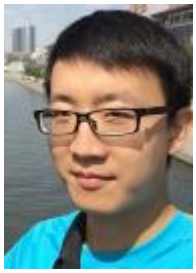
I bet that you will understand the balance of Vietnamese cuisine (and also me) when trying this food.

The rumored Bánh Xèo, a traditional vietnamese pancake. One more thing to add to the post-COVID list. (Photo:cdn.pixabay.com)

Ha's main supervisor Belén Martín-Matute (SU), and co-supervisors Rubén Martín (ICIQ), and Chad Elmore (AZ).

Yunfei Bai

ESR #4
HT



Yunfei obtained his Master's Degree from Tianjin University, China. In his spare time, he enjoys playing basketball and collecting HiFi equipment.

Why did you join CO_2PERATE?

I think the most fascinating part of the CO_2PERATE project is the cooperation between universities, companies as well as researchers of different backgrounds and research interests. Investigation of capture and utilization of CO_2 is an urgent task for both academia and industry fields.

Therefore, interdisciplinary ideas and communications are extremely important. As an industrial PhD student in CO_2PERATE project, I could have opportunities to learn from top laboratories of universities and companies, and I also think I could benefit greatly from this experience for my personal development.

Early-stage Researchers

The Haldor Topsøe building in (Ravnholm) in contrasts. (Photo: Y. Bai)

What is your project about?

My project aims at developing new chemical processes of industrial relevance using CO_2 as a reactant. The project will focus on reactions where a C-C bond is formed between CO_2 and a co-reactant as well as where CO_2 is being activated by a Lewis acid catalyst. Reactions involving C-O bond formation will be also considered, but with a lower priority. Both gas phase and liquid phase reactions will be evaluated, and the ambition is to use Lewis acidic zeolites as catalysts for the reactions.

Tell us about the institution/country you are currently in.

I am at Haldor Topsøe, Denmark. It is a beautiful country, and you can always find splendid parks and coastlines almost everywhere. We have a superb working environment in Top-søe. I work in the R&D department of biobased chemicals, and you can always establish connections with other departments easily. Here we have experts of catalyst synthesis, characterization, calculation, etc, and I have learnt a lot from them. Furthermore, employee care and safety awareness here deeply impress me.

Yunfei's main supervisor Esben Taarning (HT), and his co-supervisors Ainara Nova (UiO) and Troels Skrydstrup (AU).

Early-stage Researchers

Jhonnatan Carvalho de Oliveira Gomes

ESR #5
UiT

Jhonnatan has obtained his Master's Degree from the Federal University of Juiz de Fora, Brazil. In his free time, he enjoys singing, cooking, and playing computer games.

Why did you join CO_2PERATE?

When I first saw the position in the CO_2PERATE consortium I immediately got very excited about the whole concept of this big European Project. Not only does CO_2PERATE an outstanding job with integrating Industry and Academia but it also deals with a very interesting topic in Chemistry, aiming to combine sustainability and green chemistry focusing on CO_2 Chemistry.

What is your project about?

My project is in Computational Chemistry focused on studying reactions and mechanisms between CO_2 and alkyl compounds utilizing cheap metal catalysts. Together with experimentalists in CO_2PERATE, I will study and try to understand how CO_2 can be inserted in biomass-derived compounds to yield products that are widely used in our day-to-day life. At the moment, I'm working with Julien, sitting in Spain, on a CO_2 insertion reaction in alkyl bromides using nickel catalyst.

Northern lights shows are right outside the window when in Tromsø. (Photo: J. Carvalho)

Tell us about the institution/country you are currently in.

The University of Tromsø (UiT) is the northernmost university in the entire world. It is located in the Arctic part of Norway and despite the cold weather, people at UiT are very warm and welcoming. During my settling in time, I got huge amount of support from the university staff, as well as Kathrin and Marie from CO_2PERATE.

The postgraduate employees are very nice and this exchange between different areas within Computational Chemistry is good. Norway is an incredible country and offers a lot in terms of nature scenarios. Living in Tromsø has made me adapt myself to very different conditions from my home country, like tons of snow. It is amazing to be in close contact wherever I go with nature and especially get to see the northern lights so often. I surely enjoy the structure of UiT and Tromsø and I can't wait to experience more of what this whole experience will provide.

Jhonnatan's main supervisor Kathrin H. Hopmann (UiT), and co-supervisors Luca Frediani (UiT) and Per-Ola Norrby (AZ).

Doriane Chauvin

ESR #7
UZH

Doriane has a double Master's degree from the Chemistry School of Strasbourg and the University of Strasbourg, France. In her spare time, she enjoys playing badminton as well as other racket sports. She practices ukulele and violin every week.

Why did you join CO_2PERATE?

I have always been keenly interested in catalysis and organometallic chemistry. Joining the CO_2PERATE ITN was a singular opportunity to gain an expertise in these areas while addressing the actual need of greener solutions. I'm glad to take part in this vibrant project aiming to move towards a more sustainable chemistry. Last but not least, CO_2PERATE promotes the collaborations between institutions all

Zürich under the snow. (Photo: D. Chauvin)

across Europe, gathering both industry and academy. This multi-cultural network provides an excellent environment with high level training to push the boundaries of science.

What is your project about?

The project is focused on the development of novel catalysed transformations. We aim to use gold complexes to efficiently capture CO_2 and incorporate it into valuable molecules. A special attention is devoted to ligand design and mechanistic studies through the isolation of organometallic intermediates.

Tell us about the institution/country you are currently in.

Switzerland is a wonderful country to explore with gorgeous landscapes

The bespoke mountain landscape of Switzerland. (Photo: D. Chauvin)

(paradise for mountain lovers), a fascinating culture, and high life quality. Recently, we were lucky to have a thick layer of snow all over the city (see pictures). In a nutshell, this is the perfect place to combine chemistry, skiing hiking, fondue and much more.



Doriane's main supervisor Cristina Nevado (UZH),and co-supervisors Belén Martín-Matute (SU) and Esben Taarning (HT).

Stephanie Ton

ESR #9
AU

Stephanie obtained her Master's Degree from the University of Ottawa, Canada. In her free time, she enjoys physical activities such as yoga and running as well as baking.

Why did you join CO_2PERATE ?

I joined CO_2PERATE to be able to pursue my ambitions of participating in

high level research and contributing to the scientific community. Interactions with scientists within the CO_2PERATE ITN network as well as those at Aarhus university will provide me with invaluable opportunities to discuss findings and develop cross-disciplinary collaborations. This research network stood out to me as innovative, providing us as PhD students the opportunity to attend research secondments in both industrial and academic settings.

What is your project about?

The goal of my project is to develop novel chemistry for the efficient and late-stage incorporation of carbon isotopes into bioactive molecules. Carbon isotope labelling is an important application, as isotopically labelled pharmaceuticals are required for drug metabolism and pharmacokinetics (DMPK) studies as well carbon-11 with its short half-life in minutes, can be utilized for PET imaging. Our goal has been to implement organometallic complexes as stoichiometric reagents for the fast and efficient incorporation of the isotope-label. Currently the project is focused on a nickel-mediated carbonylative coupling for the late-stage incorporation of labelled ester functionalities.

Tell us about the institution/country you are currently in.

For my PhD I have had the opportunity to move to Aarhus, Denmark, attending Aarhus university as a part of the Interdisciplinary nanoscience centre. Pursuing a PhD in Denmark has been rewarding, along with my ambitions of joining a world-class research group, I have been able to experience and enjoy another culture. This has included (attempting to) learn the language as well as enjoying the danish cuisine, and customs, moving abroad for my PhD studies has been an extremely rewarding personal venture.

Stephanie's main supervisor Troels Skrydstrup (AU), and co-supervisors Rubén Martín (ICIQ) and Malvika Sardana (AZ).

Early-stage Researchers

Mahika Luthra

ESR #10
UiO

Mahika obtained her Master's Degree from the Indian Institute of Technology Roorkee, India. She relaxes in her spare time, reading novels and watching television series.

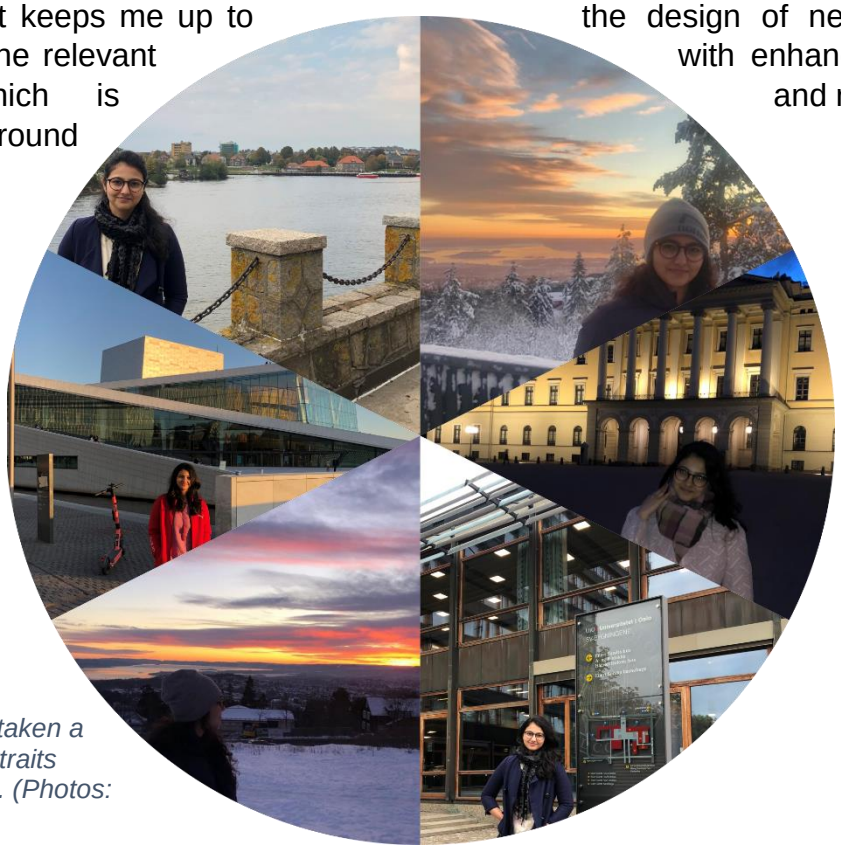
Why did you join CO_2PERATE?

I joined CO_2PERATE because of its interdisciplinary nature with different collaborations. To work in an environment, which has collaborations from different groups from different countries is what I was looking for because it not only expands my knowledge but keeps me up to date with all the relevant research which is going on around CO_2.

What is your project about?

The project focusses on processes that use CO_2 to form new C-C bonds, via CO or other intermediates, using MOF supported molecular catalysts.

Our goal will be to get a better understanding of the mechanism of these reactions and be able to develop/design new systems. The project employs high-level computational methods, including both quantum mechanics and ab initio molecular dynamics, to study non-precious metal catalysts for the formation and incorporation of CO. These catalysts will be combined within nano porous MOF materials, aiming at the design of new systems with enhanced activity and robustness.



Mahika has taken a series of portraits around Oslo. (Photos: M. Luthra)

Tell us about the institution/country you are currently in.

I am currently working in University of Oslo, Norway. Apart from its prestigious standing in academics, it provides a lot of opportunities for social interaction and activities.

As a country, Norway is beautiful with its Fjords, islands, and what not. I have had a wonderful time strolling in Drøbak, Holmenkollen, Bygdøy island, Opera house, etc (see pictures) and it was a great experience. The beauty of this country never made me feel homesick. I am looking forward to visiting other places as well in holidays.

Tell us one thing about you that you would like others to know.

I am a cheerful and friendly person, who likes to meet new people with different backgrounds. I love binge watching TV series. You would often find me discussing about classical dance and music, since I am a big fan of that.

Mahika's main supervisor Ainara Nova (UiO), and her co-supervisors Michele Cascella (UiO), Esben Taarning (HT) and David Balcells (UiO).

Julien Lyonnet

ESR #11
ICIQ

Julien obtained his Master's Degree from Uppsala University, Sweden. In his free time, he enjoys skiing, practicing kickboxing and playing the guitar.

Why did you join CO_2PERATE?

When I was looking for a PhD position, I ended up on an advertisement for the project, I am currently doing as part of CO_2PERATE. The project, involving catalysis and CO_2 chemistry, directly seemed really interesting to me. Being a Marie Curie ITN, I really like the fact that there would be planned secondments, especially in the industry. This project therefore appeared to me as a really suitable position!

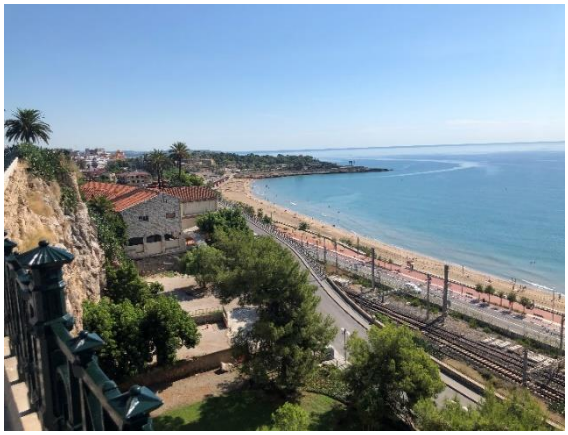
What is your project about?

My project consists of developing new catalytic strategies in order to

implement CO_2 within organic molecules with use of it as a reagent. Once such strategies have been developed, I will be tackling the use of isotopically enriched CO_2 (by mean of carbon 13 or 14) for molecular labelling.

Tell us about the institution/country you are currently in.

I am doing my project at the ICIQ, part of the University Rovira i Virgili in Tarragona, Spain. This institution is definitely part of the best in which one could imagine working at. The facilities are just incredible, and we are constantly surrounded by talented people.



Julien aslo gets to enjoy the Platja del Miracle. (Photo: J. Lyonnet)

View from the lab as the sun sets in Tarragona, Spain. (Photo: J. Lyonnet)

Spain as a country is definitely a place in which the climate is really appreciable from the autumn to the spring! It is sunny most of the time and with good temperatures even in January. Coming from a mountainy place (Geneva), living by the sea is something that I am definitely not used to but is quite pleasant. I must say that I am not particularly waiting for the summer as it will most likely be a bit too warm for me. Nevertheless, I am really enjoying my time here thanks to the people, the place and also the amazing chemistry that I am being involved with!

Julien's main supervisor Rubén Martín (ICIQ), and his co-supervisors Troels Skrydstrup (AU) and Markus Artelsmair (AZ).

Early-stage Researchers

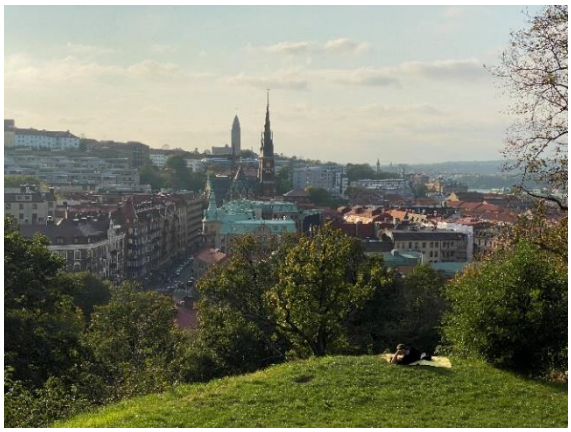
Kim Saskia Mühlfenzl

ESR #12
AZ

Kim obtained her Master's Degree from the Ludwig-Maximilians University (LMU) Munich, Germany.

Why did you join CO_2PERATE?

I joined CO_2PERATE because it offers a great opportunity to investigate the use of CO_2 as a carbon synthon for sustainable syntheses. Moreover, CO_2PERATE gives me the opportunity to gain experience of different working environments through secondments to several research institutions. In addition, the ITN enables the cooperation between industry and academia. Working at AstraZeneca allows me to gain knowledge and hands-on experience in various medicinal chemistry and drug discovery applications at the forefront of biomedical research and development.



The city of Gothenburg. (Photo: K. S. Mühfenzl)

What is your project about?

My PhD project focuses on the development of late-stage and rapid carboxylation techniques with $^{14}CO_2$ in drug development programs. The use of (labelled) COgen, which can be synthesized from (labelled) CO_2, and/or the direct use of (labelled) CO_2 could lead to a green and easily accessible alternative for the late-stage isotopic labelling of pharmaceutically relevant compounds.

Lake Delsjön in the fall and winter. (Photo: K. S. Mühfenzl)

These compounds can be further used for the study of metabolism and pharmacokinetic profiles in drug development.

Tell us about your institution/country you are currently in.

AstraZeneca is a global, innovation-driven biopharmaceutical company that focuses on the discovery, development and commercialization of prescription medicines for some of the world's most serious diseases. More than 2,400 employees from 50 countries work on the Gothenburg site (Sweden) to support the entire life cycle of AstraZeneca medicines, from drug discovery and clinical trials, to global commercialization and product maintenance.

Sweden is the third largest country in the European Union and is home to 10.4 million inhabitants, most of whom live in the three largest cities: Stockholm, Gothenburg and Malmö. Besides their fika (coffee break with pastries), during which the main topic is often the weather, Swedes love spending time in nature. Throughout the country there are numerous lakes. These are perfect for swimming in the summer and skating in the winter.

Kim's supervisor main Chad Elmore (AZ), and her co-supervisors Annette Bayer (UiT) and Troels Skrydstrup (AU).

Weiheng Huang

ESR #13
LIKAT

Weiheng obtained his Master's Degree from the Université de Rennes 1, France. In his spare time, he enjoys swimming, cycling and indoor activities such as watching animation, listening to music and playing computer games.

Why did you join CO_2PERATE?

I joined CO_2PERATE for my science interest in CO_2 reactions with organo-metallic catalysts. CO_2 chemistry is one of the most attractive topics which is highly relative to our environment and future. By this opportunity, I hope I can make a contribution applying my knowledge in such a great platform.

Early-stage Researchers

What is your project about?

My project is mainly about the alkoxy carbonylation of olefins using CO_2 instead of CO. Except replacing CO, we are developing more sustainable homogeneous organometallic catalyst using earth abundant metals such as iron or cobalt.

Tell us about the institution/country you are currently in.

I am working in Leibniz-Institut für Katalyse e.V. (LIKAT), Rostock, Germany. LIKAT is one of the largest publicly funded catalysis institutes in Europe and occupies a place at the interface between fundamentals and applications. The main focus is on application-oriented basic research and promotes industrial implementation.

Weiheng's main supervisor Matthias Beller (LIKAT), and co-supervisors Cristina Nevado (UZH) and Robert Franke (EV).

Martina Perlog

ESR #15
LIKAT

Martina obtained her Master's degree from the University of Zagreb, Croatia. In her free time, she enjoys going to the beach and spending time with friends. She also likes to watch TV series and paint.

Why did you join CO_2PERATE?

I joined the CO_2PERATE Project because solving CO_2 problem is really a crucial thing in industry and in the world, so I wanted to participate in this kind of project and learn something new. In this project I also liked that there is a lot of partners from the Nordic countries which already are running the project for utilization of CO_2, so I thought this one would be a good project too.

What is your project about?

Within the CO_2PERATE project I will work on the development of catalysts for amino carbonylation reactions of olefins with CO_2. My work in the beginning consists of synthesizing heterocyclic phosphines and preparation of cobalt complexes, and for comparison, also Pd and Ru complexes. Within my project I will also evaluate the catalytic activity in the reforming process of amines and CO_2 and test the active systems in the benchmark reaction of

Early-stage Researchers

CO_2 with olefins and amines with focus on optimization of reaction conditions and evaluation of substrate scope. When all this will be done, I will work on developing a scalable process.

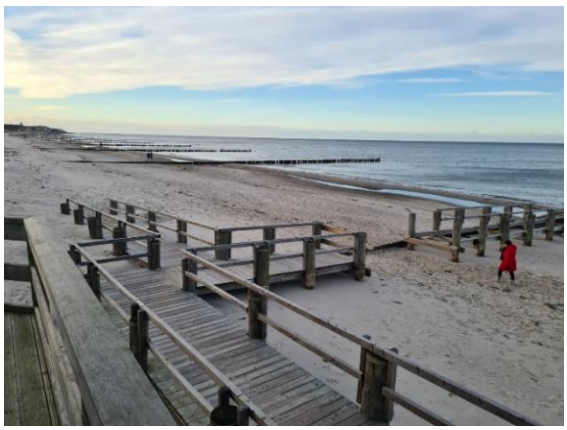
A planed secondment for my project is to Norway with Dr. Nova where I will learn to perform computational mechanistic studies so that I can gain the knowledge of mechanistic aspects. The industrial secondment is with Evonik and Prof. Franke so I could develop a scalable process.

Tell us about your institution/country you are currently in.

The Leibniz Institute for Catalysis (LIKAT) is one of the largest publicly funded research institute in the field of applied catalysis in Europe. It is an organizationally and legally independent research institute with around 300 employees and guests. The main areas of interest of the LIKAT are homogeneous and heterogeneous catalysis. Their expertise involves the development of methodology as well as application engineering.

Martina's supervisor Matthias Beller (LIKAT), and her co-supervisors Ainara Nova (UiO) and Robert Franke (EV).

The Leibniz Institute for Catalysis (LIKAT). (Photo: LIKAT)



The beach of Kühlungsborn. (Photo: M. Perlog)

I really like Rostock and the beaches around Rostock, the city is big, but not so big, traffic is okay and people in the traffic are really nice.

The city of Rostock, River Warnow and City port. (Photo: Eplisterra)


CO2