NordCO$_2$

The Nordic Consortium for CO_2 Conversion

Biannual Report 2020-2021

NordCO$_2$ – Nordic Consortium for CO$_2$ Conversion
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The Nordic Consortium for CO_2 Conversion

NordCO$_2$ is a Nordic University Hub created in 2018 to promote and enhance collaborations between researchers working on chemical CO_2 conversion in the Nordic countries. The consortium is funded by NordForsk with over 21 million NOK for the period 2018-2023.

The consortium unites 9 universities from 5 Nordic countries: UiT The Arctic University of Norway (UiT, Norway), University of Oslo (UiO), University of Bergen (UiB), Stockholm University (SU, Sweden), KTH Royal Institute of Technology (KTH), Uppsala University (UU), Aarhus University (AU, Denmark), University of Iceland (UoI, Iceland) and Helsinki University (HU, Finland). At these institutions, 12 research groups participate in the consortium, contributing their unique expertise on CO_2 conversion. Such expertise encompasses the fields of homo- and heterogeneous catalysis, by both experimental and theoretical chemists.

UiT The Arctic University of Norway

UNIVERSITY OF OSLO

UNIVERSITY OF BERGEN

HELSINGIN YLIOPISTO

KTH VETENSKAP OCH KONST

Stockholm University

AARHUS UNIVERSITY

UNIVERSITY OF ICELAND

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NordCO$_2$ Annual Report 2020-2021

Contents

Overview

One of the main missions of NordCO$_2$ is promoting the collaboration between research groups of the Nordic countries working on CO$_2$ conversion reactions. This is achieved by investing most of our funding to arrange activities and to promote the mobility of students between Nordic Universities with the aim of learning new techniques and expanding their network. Having this in mind, one can easily guess how harmful the mobility restrictions due to COVID-19 were to our consortium. As you will read in the following pages, many of the activities that were initially planned in 2020 and 2021 had to be cancelled or replaced by digital events. The latter decision was not easy because of the uncertainty on the restrictions. Also, the work load and fatigue of many PIs increased significantly during this period because they had to adapt to remote online teaching and supervision. For students, the situation was not better because of their social needs. A good example is the experience of Faranak (you can read about it in the report), who joined the group of Prof. Timo Repo during the full lockdown. These circumstances prompted us to publish a bi-annual report with the activities of 2020 and 2021, in a wish to put together the negative impact of COVID-19 with the solutions we found to keep our network alive until we could meet physically at the end of 2021. In a way, we want to isolate this period hoping that it does not happen again.

Despite the negative impact of COVID-19, we managed to produce good science and keep some collaborations digitally. In 2020 and 2021, our groups published 33 papers on topics related to CO$_2$ conversion, 6 of them involving different NordCO2 nodes. In the field of CO$_2$ conversion to chemicals, several groups focused on understanding and optimizing the formation of C-C bonds using carboxylation and carbonylation reactions. Though some of these studies still use Pd complexes, there is a clear direction towards making these processes more sustainable by using base metals such as Cu and Ni, as well as sustainable solvents and sunlight as energy source. Several groups are also working on the electroreduction of CO$_2$ to CO, formic acid and methanol with homogeneous and heterogeneous catalysts. One of the main goals in this field is increasing product selectivity, and some groups found that this can be achieved by using amines or water. In addition, metal organic frameworks and water were found to play a similar role on the thermal reduction of CO$_2$ to methanol.

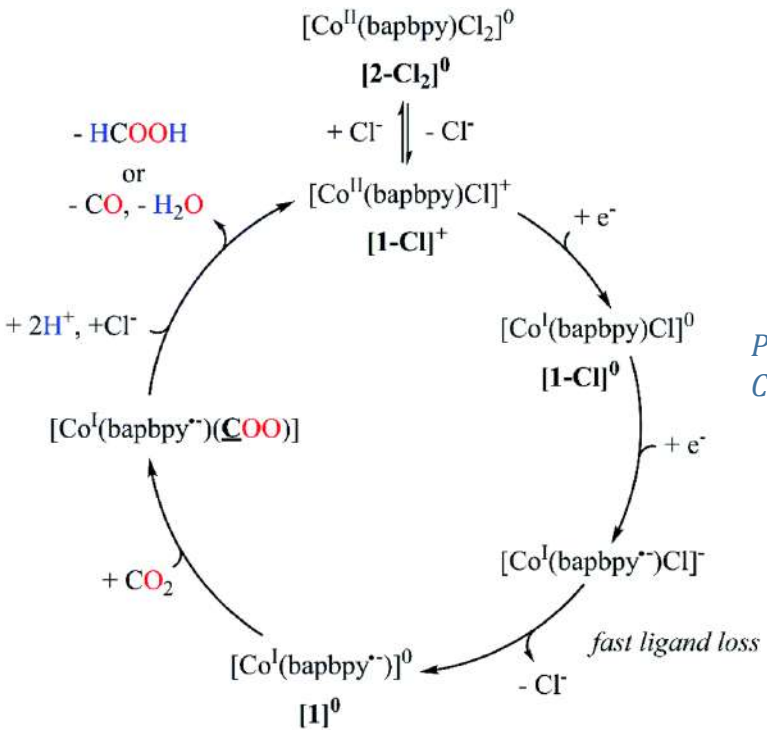
To adapt our activities to the mobility restrictions, we tested new platforms for our meetings such as Gather Town, asking the students for advice. This resulted to be extremely useful. Indeed, one of the activities we are most proud of, the $NordCO_2$ monthly seminars, came from their wish to meet regularly, having the opportunity to communicate their science. Students have also been critical with the organization of some of the activities, which we appreciate as useful feedback for further improvement. Even though digital meetings have been beneficial and will be used also in the future, one of my best 2021 experiences was to participate in the first physical meeting after the lockdown period: the $NordCO_2$ annual meeting that took place in Oslo. It was extremely satisfying to see the high motivation of people to interact with others and discuss about science.

After the covid-19 experience, we have learnt to be flexible when looking at the activities initially planned. But this does not mean that we do not have plans for the future. Indeed, for the next two years, we will continue with the online $NordCO_2$ seminars and we will meet physically at least twice a year, for both our annual meeting and one school. We have already dates and location for most of these activities (9-11/5/2022 Summer school in Bergen, 15-19/8/2022 Annual meeting in Iceland; 24-27/4/2023 Annual meeting in Finland), and a school on CO_2-to-chemicals is being planned for 2023.

Finally, I would like to thank all $NordCO_2$ PIs, PhD students, postdocs, researchers and collaborators for their great work in the difficult 2020 and 2021 years. I am also grateful to our administrator Dr. Marie-J. H. Halsør, for doing much more than administrating, taking care of our twitter account, our webpage, assist on the organization of events and gathering information and contributing in the writing of the annual and scientific reports.

Associate Professor Ainara Nova
Consortium Leader
University of Oslo
University of Tromsø

Research



Proposed mechanism for the reduction of CO_2 using [1-Cl]+ as an electrocatalyst.

N. Queyriaux, K. Abel, J. Fize, J. Pécaut, M. Orio and L. Hammarström (2020).

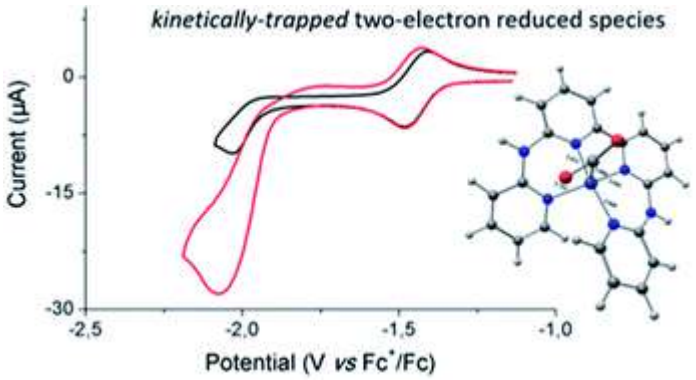
Research highlight from Uppsala University: Electro-assisted reduction of CO_2

A cobalt(II) polypyridyl complex [Co(bapbpy)Cl]+, previously reported as an active catalyst for electro-assisted H2 evolution, also proved reactive for CO2 electroreduction. Using a combination of electrochemical tools, UV-vis spectroscopy and DFT calculations, we evidenced that the second electron required over the catalytic cycle is unambiguously located within the bapbpy ligand platform.

This propensity to store electrons, however, appears detrimental to the catalytic activity by preventing effective charge delocalization into the bound CO_2 substrate. Although activated, the CO_2 molecule remains poorly reactive towards oxide acceptors, therefore limiting turnover frequency. While the potential of redox-active ligand in multi-electrons/multi-protons catalysis has often been highlighted, this study shows that the use of such ligand can be a double-edge sword as it can alter the metal-based reactivity.

Reference

N. Queyriaux, K. Abel, J. Fize, J. Pécaut, M. Orio, and L. Hammarström (2020). From non-innocent to guilty: on the role of redox-active ligand in the electro-assisted reduction of CO_2 mediated by a cobalt(II)-polypyridyl complex. *Sustainable Energy & Fuels* 4, 3668-3676.
DOI: 10.1039/D0SE00570C



$[Co(bapbpy)Cl]^+$ $[1\text{-}Cl]^+$ is a pentacoordinated polypyridyl cobalt(II) complex containing a redox-active tetradentate ligand (bapbpy: 6,6′-bis-(2-aminopyridyl)-2,2′-bipyridine). Under a CO_2 atmosphere, cyclic voltammograms of $[Co(bapbpy)Cl]^+$ exhibit significant current enhancement assigned to CO_2 catalytic reduction.

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NordCO_2 Principal Investigator Leif Hammarström is heading the research group at Uppsala University.

Research highlight from Stockholm University:

Hypervalent Iodine(III) Mediated Umpolung Coupling of CO_2 with Nucleophiles

Following their interest in the use of CO_2 as C1 building block and on the development of umpolung strategies for organic chemistry, the group of Prof. Martín-Matute at SU is currently studying the synthesis of organic carbamates by reacting a variety of nucleophiles with carbamate anions.

The transformation involves the interaction of two nucleophiles and can therefore only be achieved via an umpolung strategy. This was successfully achieved by using a hypervalent iodine(III) reagent, which induces a reverse polarity in one of the nucleophiles (manuscript in preparation).

Using this unprecedented protocol, they can react silyl enol ethers and 1,3-dicarbonyl compounds with carbamates, yielding α-carbamate carbonyl compounds under very mild conditions (1 bar CO_2 and room temperature). The method can be applied to a large number of secondary amines, which affords oxoalkylcarbamates in good yields.

The mechanism of the reaction is current being investigated by Density Functional Theory (DFT) calculations.

References:

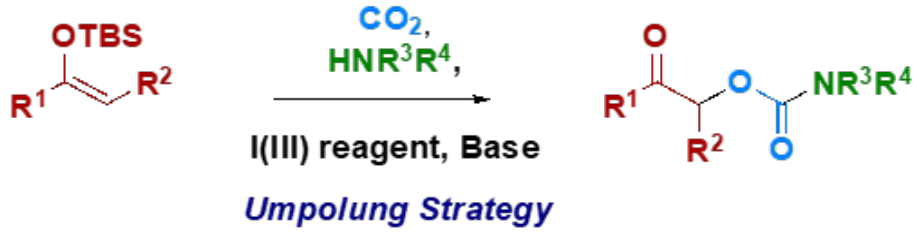
Carrasco, S., Sanz-Marco, A., Martín-Matute, B. (2019). Fast and Robust Synthesis of Metalated PCN-222 and Their Catalytic Performance in Cycloaddition Reactions with CO_2. *Organometallics* 38, 3429.
DOI: 10.1021/acs.organomet.9b00273

A. Sanz-Marco, S. Martinez-Erro, M. Pauze, W. Gómez-Bengoa, B. Martín-Matute (2019). An umpolung strategy to react catalytic enols with nucleophiles. *Nature Commun*. 10, 5244.
DOI: 10.1038/s41467-019-13175-5

S. Arava , J. N. Kumar, S. Maksymenko, M. A. Iron, K. N.Parida, P. Fristrup, A. M Szpilman (2017). Enolonium Species-Umpoled Enolates. *Angew. Chem. Int. Ed.* 56, 2599.
DOI: 10.1002/anie.201610274

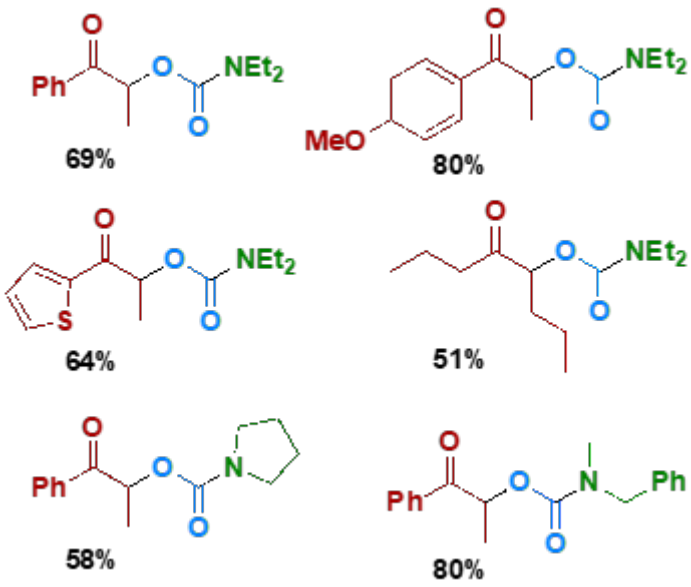
Y. Peng, J. Liu, C. Qi, G. Yuan, J. Lib, H. Jiang (2017). nBu4NI-catalyzed oxidative cross-coupling of carbon dioxide, amines, and aryl ketones: access to O-β-oxoalkyl carbamates. *Chem. Commun.* 53, 2665.
DOI: 10.1039/C6CC09762F

V. García-Vázquez, A. Carretero Cerdán, A. Sanz-Marco, E. Gómez-Bengoa, B. Martín-Matute (2022). An Expedient Method for the Umpolung Coupling of Enols with Heteronucleophiles. *Chem. Eur. J.* 2022.
DOI: 10.1002/chem.202201000



The umpolung coupling of CO_2 with silyl enol ethers.

Examples of oxoalkylcarbamates obtained from secondary amines using the umpolung strategy, with their respective yields.

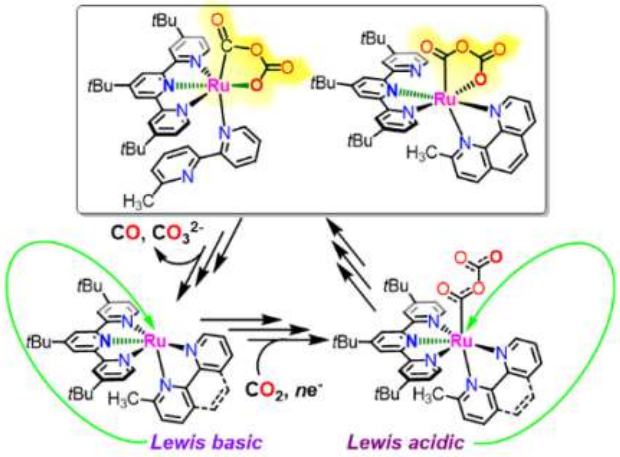


The members participating in this research are V. García Vásquez, A. Sanz-Marco and B. Martín-Matute.

Research highlight from Uppsala University & KTH Royal College of Technology:

Exploring the mechanism for homogeneously catalysed reduction of CO_2 to CO

Over the last year we have dug deeper into the mechanism of CO_2 to CO conversion, catalyzed electrochemically by $[Ru(tBu_3tpy)(pp)(CH_3CN)]^{2+}$ catalyst framework (*pp* = bidentate polypyridyl ligand) in the absence of an external acid source. This work is inspired by previous reports of such catalysts from the group of NordCO$_2$ PI Prof. Sascha Ott (UU), and is the result of an ongoing fruitful collaboration between the NordCO$_2$ groups at UU and KTH.



Electroreduction of CO_2 to CO using a polypyridyl ligand.

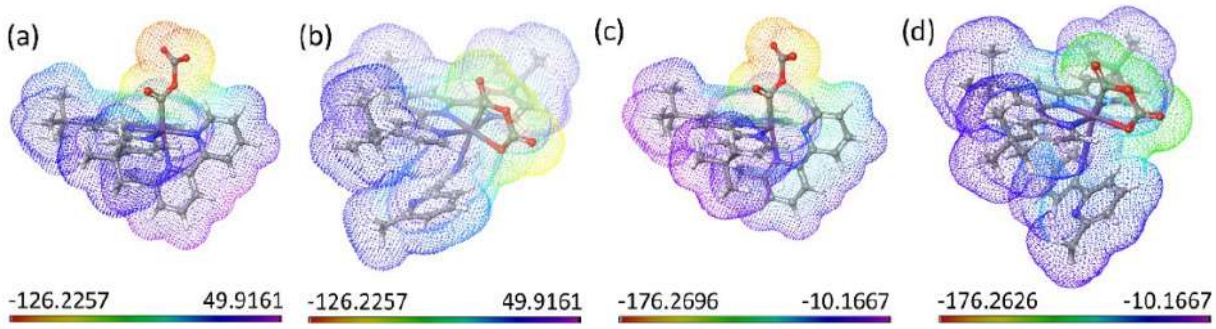
In the course of our study we have discovered a yet unprecedented $[Ru\text{-}CO_2CO_2]^{0,c}$ metalacyclic intermediate in the low overpotential reaction pathway for electrocatalytic CO_2 reduction. Metalacyclic intermediates of this kind exist in a few earlier reports, however, they were all synthesized by stoichiometric activation of CO_2. The combination of density functional theory (DFT) calculations and spectroscopic experiments has led us to decipher a unique role played by the ruthenium center, whose ability to be electronically fine-tuned allows it to display both nucleophilic (attacks the C center of CO_2) and electrophilic (coordinates to negatively charged O of CO_2) properties, at different stages of the catalytic cycle. This special property of the metal, along with the structural flexibility of the polypyridyl (*pp*) ligands aiding in their partial decoordination-recoordination on the metal, is what leads to the formation of the aforementioned cyclic intermediate by intramolecular cyclization. We show by DFT calculations that this intermediate is crucial for C-O bond-breaking, as it undergoes a third reduction at a potential that is more positive than that of the first reductions, resulting in a $[Ru\text{-}CO_2CO_2]^{-1,c}$ metalacyclic intermediate.

A new catalyst synthesized by smart choice of the *pp* ligand, has allowed us to trap these intermediates by kinetically slowing down the C-O bond dissociation step. We have characterized these intermediates by spectroscopic techniques like FT-IR and NMR on aliquots withdrawn from reaction solutions during controlled potential electrolysis using isotopically labelled $^{13}CO_2$. The spectral signatures are corroborated by DFT calculations.

Further mechanistic studies on this catalytic framework are ongoing at both UU and KTH.

Reference

Agarwala, Hemlata; Chen, Xiaoyu; Lyonnet, Julien R.; Johnson, Ben A; Ahlquist, Mårten; Ott, Sascha (2021). Alternating substrate/ligand-metal coordination enables a lowenergy pathway for C-O bond cleavage in the electrocatalytic reduction of carbon dioxide. *ChemRxiv.* Preprint.
DOI: 10.26434/chemrxiv.14035625.v2



Plots of electrostatic potentials mapped onto electron density for (a) $[1\text{-}CO_2CO_2]^0$, (b) $[1\text{-}CO_2CO_2]^{0,c,}$ (c)$[1\text{-}CO_2CO_2]^{-1}$ and (d) $[1\text{-}CO_2CO_2]^{-1,c}$. The values on the colour bars correspond to the range of electrostatic potentials (in kcal mol^{-1}); iso-value for electron density = 0.001 e $Bohr^{-3}$.

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KTH VETENSKAP OCH KONST

$NordCO_2$ members who are a part of this project: H. Agarwala (UU), X. Chen (KTH), M. Ahlquist (KTH), S. Ott (UU).

Research highlight from University of Bergen:

Computational Studies of Iron Porphyrin and Zinc Bacteriochlorin

During the last year, we have been investigating iron porphyrin and zinc bacteriochlorin in homogeneous electrocatalytic reduction of CO_2 to CO. The iron porphyrins are one of the most interesting catalysts in this regard, as it has shown state-of-the-art activity and low overpotential. Zinc bacteriochlorin, a new candidate, does not fall far behind and has also better stability and stands out as an interesting study.

The central research question has been: What roles does the metal and ligand play? We are the first group to do a direct comparison of the two promising catalysts. Our computational results have agreed with experiments, revealing that both the metal and ligand have different roles to play. The energetic landscape of the reaction is quite different for the iron and zinc systems, where the zinc system performs worse than iron. However, the bacteriochlorin ligand remains a promising candidate.

Using the structures and energies from the DFT-investigation of the four systems, the semi-empirical tight-biding method GFN2-xTB has been validated and reproduces the structures with promising accuracy. Currently the group is taking advantage of this by using the method in meta-dynamic simulations of the iron porphyrin system to investigate substituents on the ligand, as well as the effect of the solvent, counterions and electrolyte on the CO_2 to CO reduction.

References:

C. Bannwarth, S. Ehlert, S. Grimme (2019). GFN2-xTB—An Accurate and Broadly Parametrized Self-Consistent Tight-Binding Quantum Chemical Method with Multipole Electrostatics and Density-Dependent Dispersion Contributions. *J. Chem. Theory Comput.* 15, 1652–1671.
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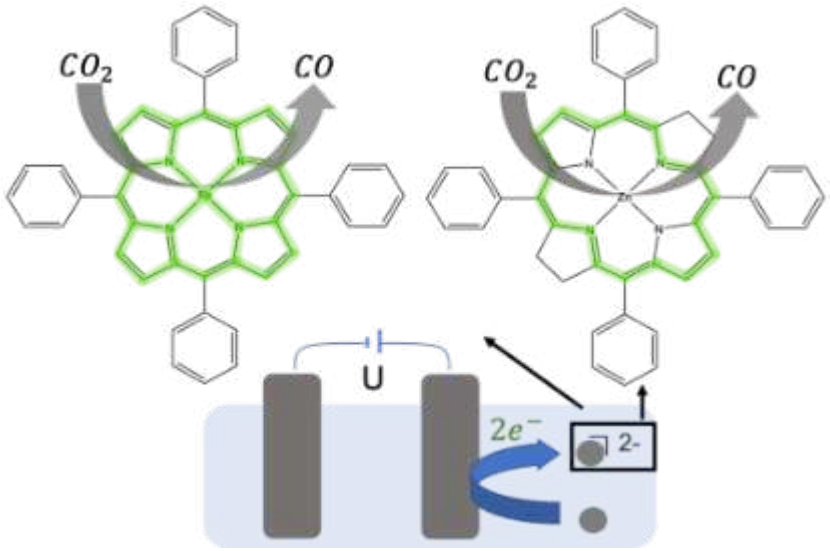
S. Grimme (2019). Exploration of Chemical Compound, Conformer, and Reaction Space with Meta-Dynamics Simulations Based on Tight-Binding Quantum Chemical Calculations. *J. Chem. Theory Comput.* 15, 2847–2862.
DOI: 10.1021/acs.jctc.9b00143



Overview of electrocatalytic reduction of CO_2 by iron porphyrin (left) and zinc bacteriochlorin (right). The marked green areas on the ligands represent the electron density stemming from the reductions.

UNIVERSITY OF BERGEN

NordCO_2 members participating in this research are K. Børve, V. R. Jensen, M. Tysse, S. H. H. Eliasson, all UiB.

Publications

As previously mentionned, the research promoted by the NordCO$_2$ consortium focuses on two main axes: the conversion of CO_2 to chemicals and pharmaceuticals and energy storage. Four projects were outlined at the time of creation of the consortium: *i) C-C bonds from CO_2*, leading to carbonyl compounds, carboxylic acids and derivatives; *ii) dimerization of CO_2 to oxalic acid* for the synthesis of ethylene glycol; *iii) electrochemical and photochemical reduction of CO_2 to CO*; *iv) incorporation of efficient catalysts into metal-organic frameworks (MOFs)*. The published output for 2020 and 2021 is presented somewhat according to these projects.

CO_2 to chemicals

To Bind or Not to Bind: Mechanistic Insights into C-CO_2 Bond Formation with Late Transition Metals. **D. García-López, L. Pavlovic, K. H. Hopmann.** *Organometallics* **2020**, 39, 1339.
DOI: 10.1021/acs.organomet.0c00090

Formal C-H Carboxylation of Unactivated Arenes. **A. Gevorgyan, K. H. Hopmann, A., Bayer.** *Chemistry-a European Journal* **2020**, 26, 6064.
DOI: 10.1002/chem.202000515

Renewable Solvents for Palladium-Catalyzed Carbonylation Reactions. **A. Ismael, A. Gevorgyan, T. Skrydstrup, A. Bayer.** *Organic Process Research & Development* **2020**, 24, 2665.
DOI: 10.1021/acs.oprd.0c00325

Exploration of New Biomass-Derived Solvents: Application to Carboxylation Reactions. **A. Gevorgyan, K. H. Hopmann, A. Bayer.** *Chemsuschem* **2020**, 13, 2080.
DOI: 10.1002/cssc.201903224

Carbonylative Suzuki-Miyaura couplings of sterically hindered aryl halides: synthesis of 2-aroylbenzoate derivatives. **A. Ismael, T. Skrydstrup, A. Bayer.** *Organic & Biomolecular Chemistry* **2020**, 18, 1754.
DOI: 10.1039/D0OB00044B

Mechanistic Insights into Copper-Catalyzed Carboxylations. **M. F. Obst, A. Gevorgyan, A. Bayer, K. H. Hopmann.** *Organometallics* **2020**, 39, 1545.
DOI: 10.1021/acs.organomet.9b00710

Mechanistic study on the regioselective Ni-catalyzed dicarboxylation of 1,3-dienes with CO_2. **W. Nie, Y. F. Shao, M. S. G. Ahlquist, H. Z. Yu, Y. Fu.** *Organic Chemistry Frontiers* **2020**, 7, 4080.
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DOI: 10.1039/D1CY01433A

Computational and Experimental Insights into Asymmetric Rh-Catalyzed Hydrocarboxylation with CO_2. **Pavlovic, L., Pettersen, M., Gevorgyan, A., Vaitla, J., Bayer, A., & Hopmann, K. H.** *European Journal of Organic Chemistry*, **2021**(4), 663.
DOI: 10.1002/ejoc.202001469

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

Access to Aryl and Heteroaryl Trifluoromethyl Ketones from Aryl Bromides and Fluorosulfates with Stoichiometric CO. **M. B. Johansen, O. R. Gedde, T. S. Mayer, T. Skrydstrup.** *Organic Letters* **2020**, 22, 4068.
DOI: 10.1021/acs.orglett.0c01117

Silylcarboxylic Acids as Bifunctional Reagents: Application in Palladium-Catalyzed External-CO-Free Carbonylative Cross-Coupling Reactions. **X. Li, J. Xu, Y. Li, S. Kramer, T. Skrydstrup, Z. Lian.** *Advanced Synthesis & Catalysis* **2020**, 362, 4078.
DOI: 10.1002/adsc.202000586

Stoichiometric Studies on the Carbonylative Trifluoromethylation of Aryl Pd(II) Complexes using TMSCF3 as the Trifluoromethyl Source. **K. Domino, M. B. Johansen, K. Daasbjerg, T. Skrydstrup.** *Organometallics* **2020**, 39, 688.
DOI: 10.1021/acs.organomet.9b00849

Main element chemistry enables gas-cylinder-free hydroformylations. **S. K. Pedersen, H. G. Gudmundsson, D. U. Nielsen, B. S. Donslund, H. C. D. Hammershoj, K. Daasbjerg, T. Skrydstrup.** *Nature Catalysis* **2020**, 3, 843.
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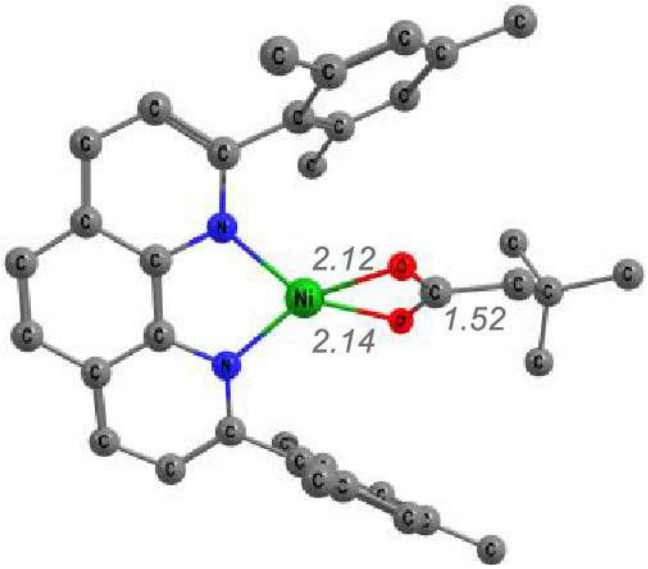
Rational selection of co-catalysts for the deaminative hydrogenation of amides. **L. A. Suarez, U. Jayarathne, D. Balcells, W. H. Bernskoetter, N. Hazari, M. Jaraiz, A. Nova.** *Chemical Science* **2020**, 11, 2225.
DOI: 10.1039/C9SC03812D

A Nickel(II)-Mediated Thiocarbonylation Strategy for Carbon Isotope Labeling of Aliphatic Carboxamides. **Pedersen, S. S., Donslund, A. S., Mikkelsen, J. H., Bakholm, O. S., Papp, F., Jensen, K. B., Gustafsson, M. B. F., & Skrydstrup, T.** *Chemistry – A European Journal* **2021**, 27(24), 7114.
DOI: 10.1002/chem.202005261



The Ni(I)–carboxylate complex synthetised by Sommerville and collaborators, in a joint paper from UiT and ICIQ, Spain.

Energy Storage

Evaluation of the Electrocatalytic Reduction of Carbon Dioxide using Rhenium and Ruthenium Bipyridine Catalysts Bearing Pendant Amines in the Secondary Coordination Sphere. **M. R. Madsen, J. B. Jakobsen, M. H. Rønne, H. Liang, H. C. D. Hammershoj, P. Norby, S. U. Pedersen, T. Skrydstrup, K. Daasbjerg.** *Organometallics* **2020**, 39, 1480.
DOI: 10.1021/acs.organomet.9b00815

From non-innocent to guilty: on the role of redox-active ligands in the electro-assisted reduction of CO_2 mediated by a cobalt(ii)-polypyridyl complex. **N. Queyriaux, K. Abel, J. Fize, J. Pécaut, M. Orio, L. Hammarström.** *Sustainable Energy & Fuels* **2020**, 4, 3668.
DOI: 10.1039/D0SE00570C

Ligand-Controlled Product Selectivity in Electrochemical Carbon Dioxide Reduction Using Manganese Bipyridine Catalysts. **M. H. Rønne, D. Cho, M. R. Madsen, J. B. Jakobsen, S. Eom, E. Escoude, C. D. Hammershoj, D. U. Nielsen, S. U. Pedersen, M. H. Baik, T. Skrydstrup, K. Daasbjerg.** Journal of the *American Chemical Society* **2020**, 142, 4265.
DOI: 10.1021/jacs.9b11806

Why do RuO_2 electrodes catalyze electrochemical CO_2 reduction to methanol rather than methane or perhaps neither of those? **E. Tayyebi, J. Hussain, E. Skúlason.** *Chemical Science* **2020**, 11, 9542.
DOI: 10.1039/D0SC01882A

Promoting Selective Generation of Formic Acid from CO_2 Using Mn(bpy)(CO)3Br as Electrocatalyst and Triethylamine/Isopropanol as Additives. **Madsen, M. R., Rønne, M. H., Heuschen, M., Golo, D., Ahlquist, M. S. G., Skrydstrup, T., Pedersen, S. U., & Daasbjerg, K.** *Journal of the American Chemical Society* **2021**,143 (48), 20491.
DOI: 10.1021/jacs.1c10805

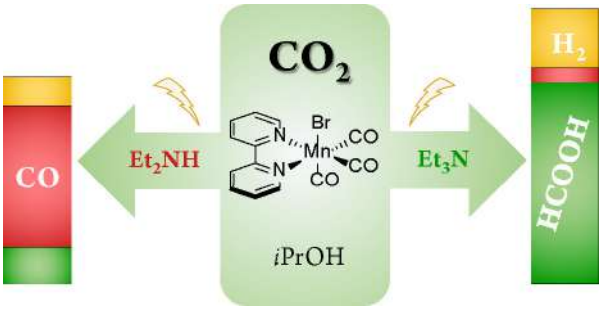
Effect of co-adsorbed water on electrochemical CO_2 reduction reaction on transition metal oxide catalysts. **Atrak, N., Tayyebi, E., & Skúlason, E.** *Applied Surface Science* **2021**, 570, 151031.
DOI: 10.1016/j.apsusc.2021.151031

Electrochemical, Spectroscopic, and Computational Investigation of a Series of Polypyridyl Ruthenium(II) Complexes: Characterization of Reduced States. **Queyriaux, N., Esmieu, C., Gupta, A. K., Vendier, L., Ott, S., Orio, M., & Hammarström, L.** *European Journal of Inorganic Chemistry*, **2021**(13), 1263.
DOI: 10.1002/ejic.202001165

Mechanistic study on the photo carboxylation of benzylic C-H bonds by xanthone and Ni(0) catalysts. **Xu, Z., Liu, D., Yu, H., Ahlquist, M. S. G., & Fu, Y.** *Molecular Catalysis* **2021**, 514, 111785.
DOI: 10.1016/j.mcat.2021.111785

Are Amines the Holy Grail for Facilitating CO_2 Reduction? **Jakobsen, J. B., Rønne, M. H., Daasbjerg, K., & Skrydstrup, T.** *Angew. Chem. Int. Ed.* **2021**, 60, 9174.
DOI: 10.1002/anie.202014255

Pivotal Electron Delivery Effect of the Cobalt Catalyst in Photocarboxylation of Alkynes: A DFT Calculation. **Xu, Y., Shao, Y., Ahlquist, M. S. G., Yu, H., & Fu, Y.** *The Journal of Organic Chemistry* **2021**, 86(2), 1540.
DOI: 10.1021/acs.joc.0c02393



Madsen and co-workers studied the reduction of CO_2 using the $Mn(bpy)(CO)_3Br$ electrocatalyst.

Hydrogenation of CO_2 to Methanol by Pt Nanoparticles Encapsulated in UiO-67: Deciphering the Role of the Metal-Organic Framework. **E. S. Gutterød, A. Lazzarini, T. Fjermestad, G. Kaur, M. Manzoli, S. Bordiga, S. Svelle, K. P. Lillerud, E. Skúlason, S. Oien-Odegaard, A. Nova, U. Olsbye.** Journal of the American Chemical Society **2020**, 142, 999.
DOI: 10.1021/jacs.9b10873

Influence of Defects and H2O on the Hydrogenation of CO_2 to Methanol over Pt Nanoparticles in UiO-67 Metal-Organic Framework. **E. S. Gutterød, S. H. Pulumati, G. Kaur, A. Lazzarini, B. G. Solemsli, A. E. Gunnaes, C. Ahoba-Sam, M. E. Kalyva, J. A. Sannes, S. Svelle, E. Skúlason, A. Nova, U. Olsbye.** Journal of the American Chemical Society **2020**, 142, 17105.
DOI: 10.1021/jacs.0c07153

Immobilizing molecular Ru complexes on a protective ultrathin oxide layer of p-Si electrodes towards photoelectrochemical CO_2 reduction. **Laurans, M., Wells, J. A. L., & Ott, S.** Dalton Transactions **2021**,50, 10482.
DOI: 10.1039/D1DT01331A

Deconstructing the Enhancing Effect on CO_2 Activation in the Electric Double Layer with EVB Dynamic Reaction Modeling. **X. Y. Chen, M. S. G. Ahlquist.** *Journal of Physical Chemistry C* **2020**, 124, 22479.
DOI: 10.1021/acs.jpcc.0c05974

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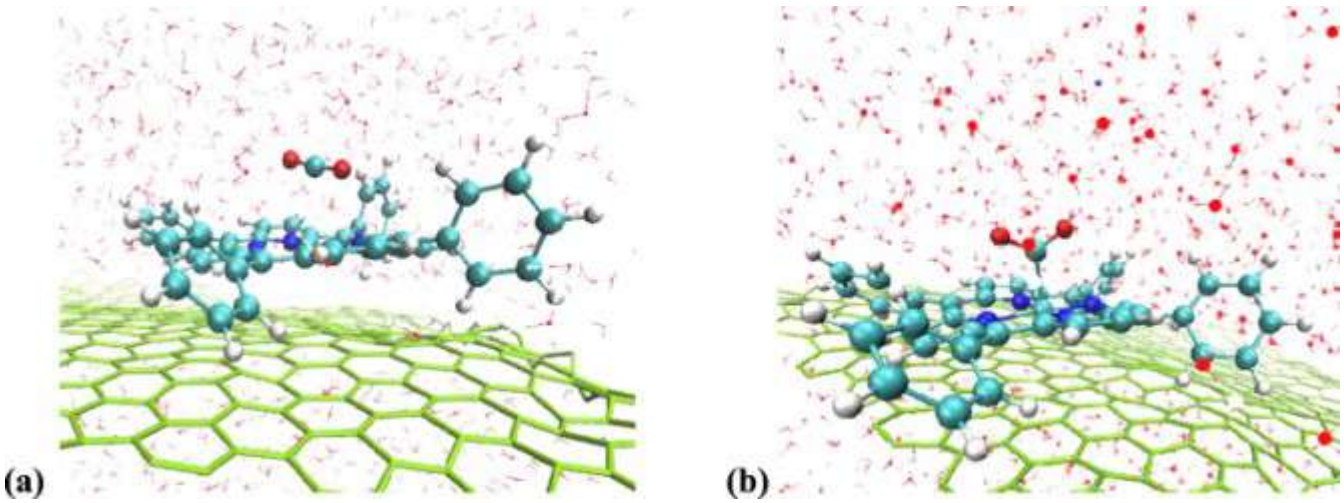
DOI: 10.1021/acs.organomet.9b00726

Computational Studies on the Mechanisms for Deaminative Amide Hydrogenation by Homogeneous Bifunctional Catalysts. **Artús Suàrez, L., Balcells, D., & Nova, A.** *Topics in Catalysis* **2021**, 65, 82.
DOI: 10.1007/s11244-021-01542-w



The $Co^{I}(TPP)^{-}$ system investigated by X. Chen and co-workers: (a) reactant state and (b) product state, both at a graphene–water interface.

Activities

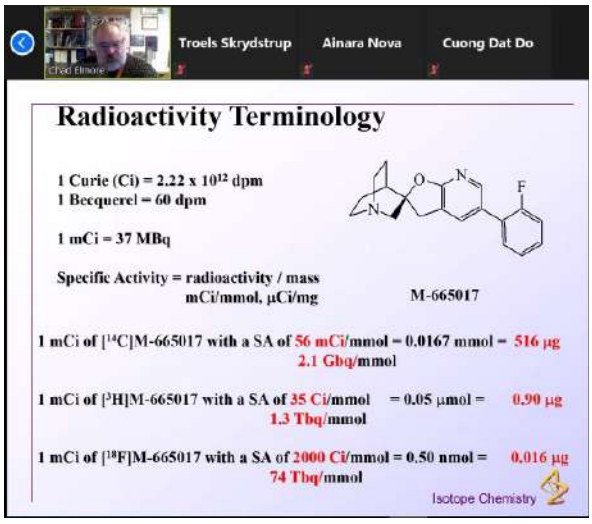
The activities of the consortium have been heavily impacted by the pandemic in 2020 and the following period of travel restrictions. The activities in 2020 were combined as a single online meeting. The same was done in 2021 , but we managed to meet physically, a first for many of our new members!

The situation also permitted us to adapt and find new ways to uphold contact: early in 2021 was the first installement of our "Monthly Seminar Series", a monthly digital seminar open to the public.

2020: Annual Meeting and Industry Panel

The 2020 Annual Meeting for NordCO$_2$, originally planned in Iceland, was held digitally from the 21st to 29th October 2020. Together with it, the Industry Panel Meeting (originally planned in Denmark) took place, with guest speakers from AstraZeneca and Haldor Topsøe. The combined meeting was organised over 5 days in two-hour sessions, each split between oral presentations from NordCO$_2$ students and talks from the guest speakers.

2020 marked the start of digital meetings with the 2020 annual meeting and Industry meeting being the firsts. These digital meetings were held as five two-hour sessions over the span of 8 days.



$NordCO_2$ PI Troels Skrydstrup launched the meeting on the 21st of October, followed by leader Kathrin H. Hopmann who gave sn update on the status of the consortium. The rest of the session was dedicated to Professor Chad Elmore from AstraZeneca (Sweden), who gave a talk titled "The use of Isotopic Carbon Dioxide in Drug Discovery".

The second and third days were split between student presentations and group activities. $NordCO_2$ students Christina Erken (Postdoc, HU), Hemlata Agarwala (Postdoc, UU), Isabelle Gerz (PhD student, UiO), Jere Mannisto (PhD student, HU), Joakim Bøgelund (PhD student, AU) and Marc F. Obst (Postdoc, UiT), gave talks about their research. The first group activity was focused on the topic of CO_2 in Industry, while the second session was used to elect the student representative for the $NordCO_2$ steering committee.

Feedback from the students about the group activities were gathered by the student representatives Liselotte Karulf (PhD student, HU) and Jere Mannisto (PhD student, HU):

"*The first activity was about the students self-assessing their reactions in industrial context, and this was to be done individually or in groups. It became apparent that many of the students were holding back, not knowing how much they can discuss their current project in $NordCO_2$ context. This meant already published work was emphasized. It is important to remind $NordCO_2$ exists to share current information among members, and thereby elevating the research to a higher level by solving problems together. Nevertheless, the students found the activity stimulating and valuable.*

The second activity was to generate questions for the industry round table, which would take place the following week. As with the first activity, more guidance would have been helpful. For example, it would have been useful to provide more context of the industrial participants. A short introduction of themselves and their needs, including their position in the company. However, the discussions were still very useful and productive, and there were produced ten questions for the round table during the first group activity."

On the 28th of October, Kristina Öhlén from AstraZeneca and Dr. Esben Taarning from Haldor Topsøe (Denmark) both gave talks on CO_2 utilization for sustainable drug purification and catalytic processes for the production of biochemicals, respectively. After that, the "Round Table" event took place, which allowed the students to ask questions (prepared during the group activity on the 22nd of October) to Prof. Skrydstrup and Dr. Taarning.

The feedback from the students was positive, although they expressed the limitations of a digital meeting for this kind of panel activity:

"*Esben Taarning and Troels Skrydstrup discussed the questions in detail the following Wednesday (28.10). Many felt the industrial panel discussion would have been even more productive in person, because it is not easy to have a critical discussion over Zoom. This is a difficult issue and we do not have a clear solution when meeting in person is not a realistic alternative. Overall, the panel discussion was very insightful, and many expressed their desire to have similar events in the future.*"

The last day consisted entirely of student presentations, including talks by Alejandro Valiente (PhD student, SU) together with CO$_2$PERATE PhD student Vu Duc Ha Phan (SU), Sri Harsha Pulumati (PhD student, UoI), and Morten Tysse (PhD student, UiB).

The event was the occasion for all to try the spatial video chat platform Gather (often referred to as Gather Town and abbreviated as GT). The format allows avatars of participants to move within interactive maps with 8-bit graphics. When avatars are close, video chat connects. The platform was used in an endeavour to promote mingling and informal discussions such as would naturally occur at a physical meeting.

S. H. Pulumati's title slide and the personal information slide for A. Valiente and V. D. H. Phan.

The comments from the student representatives concerning Gather are such:

"*On Wednesday 21.10, the first day of the Industry & Annual NordCO$_2$ Meeting 2020, it was not clear to most participants why the conference simulator program GT was used to enter Zoom. The participants needed to enter the virtual conference hall in GT to receive the link to the Zoom event. All talks were performed over Zoom, while the activities took place in the seminar room of GT. A feature of GT is that the participants' volume changes as a function of distance to other participants. Therefore, one has to move their character in order to speak with other participants. The tables in GT provide an opportunity for private conversations, as only the people around the table can hear the conversation. Unfortunately, many had technical issues at the beginning, despite being familiar with Zoom. It seemed that the challenges with GT were resolved by the third day (Friday 23.10). By this point, most participants realized the advantages of GT and wanted to implement it for their own purposes. Certainly, we expect GT to see an increase in use in the near future.*"

Monthly Seminar Series

The feedback from the students after the summer school in late 2019 mentioned their wish to have regular talks about current research relevant for the $NordCO_2$ consortium. With this as a starting point and the need to uphold activities during the pandemic, it was decided late 2020 to organise monthly digital events hosted by each node in turn. Eight seminars were held in 2021, all with more or less the same setup: a guest lecture and a student talk, for a duration of up to two hours (thus leaving ample time for discussion).

The seminars served both as a regular meeting for $NordCO_2$ members as well as outreach to the scientific community, since most of the talks were open to the public.

The advertisement for the November seminar (figure: M.-J. H. Halsør).

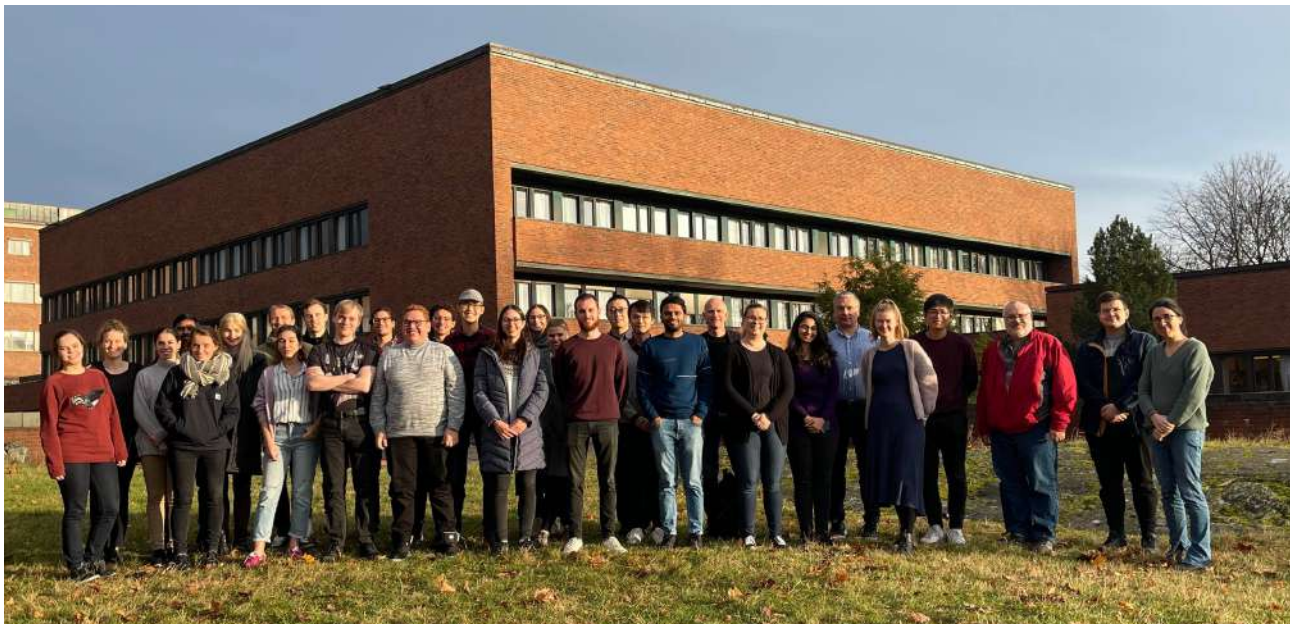
Month	Host	Guest Lecture	Student talk
March	UU	Pr. Marc Robert, Université Paris Diderot (France): "*Molecular (photo)electrochemical Reduction of CO_2 with Co and Fe Complexes*".	Simon Pedersen (AU)
April	HU	Pr. Matthias Beller, LIKAT (Germany): "*Unifying Concepts for the Development of Catalysts for Small Molecule Activation*" Prof. Walter Leitner, Max Planck Institute for Chemical Energy Conversion (Germany): "*Power-to-X catalytic conversion of carbon dioxide and hydrogen for fuels and chemicals*"	None
May	UiO	Dr. Aleix Comas-Vives, Universitat Autònoma de Barcelona (Spain) "*Theory-Aided Comprehension of CO_2 Conversion on Heterogeneous Catalysts*"	Ebrahim Tayyebi (UoI)
June	UiT	Assoc. Prof. Nina Lock (AU): "*Metal-organic frameworks for electrocatalytic CO_2 reduction*"	None
September	KTH	Pr. Julio Lloret-Fillol, ICIQ (Spain): "*Well-Defined Catalysts for Reductive Transformations; From Solar Fuels to Fine Solar Chemicals*"	None
October	UiB	Pr. James Mayer, Yale University (USA) : "*Fundamental properties of iron–porphyrin (electro)catalysts for O_2 reduction, with implications for CO_2 reduction*"	Morten Tysse (UiB)
November	SU	Pr. Liane Rossi, University of São Paulo (Brazil): "*Optimizing the selectivity of supported nickel catalysts for CO_2 catalytic hydrogenation*"	Victor García (SU)
December	UoI	Dr. Federico Calle-Vallejo, Universitat Autònoma de Barcelona (Spain)	Narges Atrak (UoI)

Winter School 2021

Finally! The first physical meeting since the beginning of 2020 gathered both NordCO$_2$ and CO$_2$PERATE members at the occasion of the Winter School 2021. The courses were focused on reaction mechanisms as well as isotopic labelling. The event was organised at the University of Oslo (UiO) from the 22nd to the 24th of November 2021 and had about 30 participants. As the majority of members are different from that of 2019, it was the first time meeting for most.

The course consisted of digital lectures in the mornings, allowing members who where not able to travel to participate. In the afternoons, practical sessions focused on group work took place. The students, who submitted reactions of interest beforehand, worked together to propose mechanisms for each other's reactions.

Students and teachers hard at work during the practical sessions (photos: M.-J. H. Halsør).



The NordCO$_2$ and CO$_2$PERATE members present at the Winter School 2021 (photo: M.-J. H. Halsør).

Annual Meeting 2021

Would it be in Iceland, would it be digital? At the end, the SC decided to take advantage of the (temporarily) loosened travel restrictions that allowed us to plan the Winter School as a physical meeting to affix the Annual Meeting 2021 to it. This allowed our members to make most of their trip to Oslo, with many taking the opportunity to stay even longer outside of the events for tourism purposes. As an exceptional gesture, CO_2PERATE members not part of NordCO_2 were invited as well, increasing their opportunities to socialise.
The event consisted in presentations from both students and Principal Investigators (PIs), a trip to Sungsvannet lake, and an evening poster session.

A well-earned dinner after a long day of courses (figure: M.-J. H. Halsør).

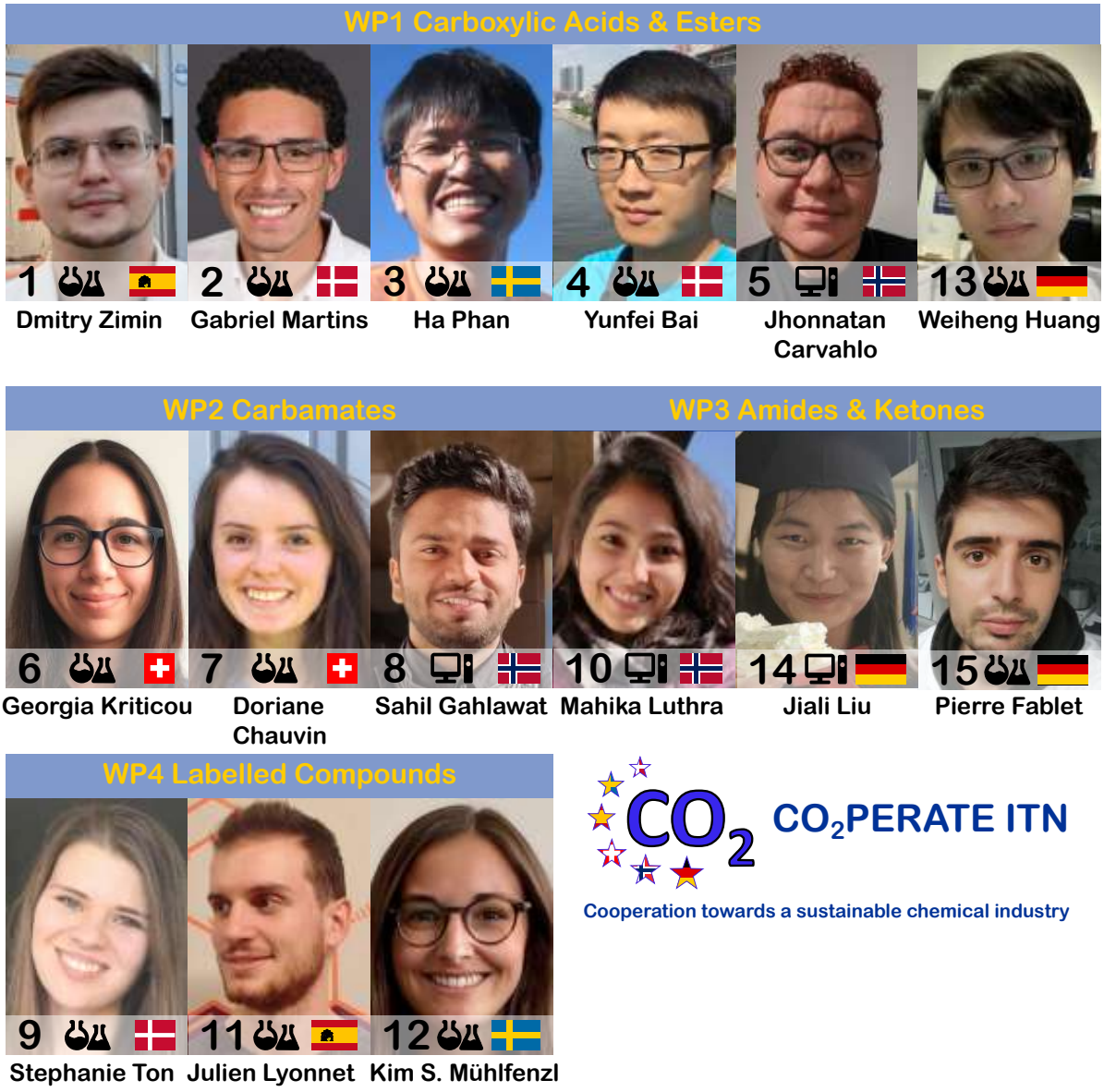
Two moments of the meeting: Researcher P. Vasko (HU) presenting aluminium as an element of interest and the intense discussions during the poster session (photos: M.-J. H. Halsør).

CO$_2$PERATE Innovative Training Network

The CO$_2$PERATE Innovative Network (ITN, Marie Skłodowska-Curie grant agreement No. 859910) was started by NordCO$_2$ PIs K. H. Hopmann, A. Bayer, A. Nova, T. Repo, B. Martín-Matute, and T. Skrydstrup, along with EAB member R. Martin (ICIQ, ES) and Prof. Matthias Beller (LIKAT, DE), Dr. Charles S. Elmore (AstraZeneca, SE), Prof. Robert Franke (Evonik, DE), Prof. Cristina Nevado (UZH, CH) and Dr. Esben Taarning (Haldor Topsoe, DK). The funding was granted in 2019 and the network officially started on the 1st of February 2020.

The ITN consists of 15 research projects on the topic of the synthesis of indispensable molecules from sustainable carbon sources and with sustainable catalysts. The projects focus on the C-C bond formation with CO$_2$ and are grouped in 4 work packages (WPs) according to the desired products (for a description of the different work packages, see our Annual Report 2019).

The 15 early-stage researchers (ESRs) part of CO$_2$PERATE, grouped by Work Package (WP). Each ESR has an attributed number corresponding to their individual project. Figure by M.-J. H. Halsør.



CO$_2$PERATE ITN

Cooperation towards a sustainable chemical industry

The main goal for the first year of the ITN was to recruit the fellows, who had to fulfil a mobility rule stating that it is not possible to enter the programme in a country where you have been residing for more than 12 months during the last 36 months at the time of enrolment. Considering that most COVID-19 related lockdowns came into effect during March 2020, it was no small feat to be able to recruit 12 early-stage researchers (ESRs) during that year. The recruitment continued in 2021. The last position (at LIKAT, Germany) used to be filled by PhD student Martina Perlog, but she left the ITN in August 2021. Pierre Fablet is replacing her since the beginning of 2022.

In addition to recruitment, the ITN management team worked on establishing the CO_2PERATE Supervisory Board, which had several meetings during 2020. The outcome of these meeting was, amongst others, the first ESR training courses that took place from the 14th to the 16th of December 2020. The topics for the courses were Open Science (1 day) as well as Responsible Research and Innovation (RRI, 2 days). The courses were hosted (digitally!) by AU (Denmark), LIKAT (Germany), and UiT (Norway).

In 2021, the CO_2PERATE students were able to participate in the NordCO_2 monthly seminars, and they had they very first physical meeting at the Winter School 2021, hosted by UiO in Oslo (Norway).

You can read more the ITN in the CO_2PERATE annual reports, available at co2perate.eu.

The CO_2PERATE PhD students at the RRI course in 2020. Also in the picture CO_2PERATE PIs Kathrin Hopmann (UIT) and Troels Skrydstrup (AU) as well as the Open Science presenters Marie Louise Conrad (AU) and Morten Hjorth Gad (AU). Photo by M.-J. H. Halsør.

Steering Committee Meetings

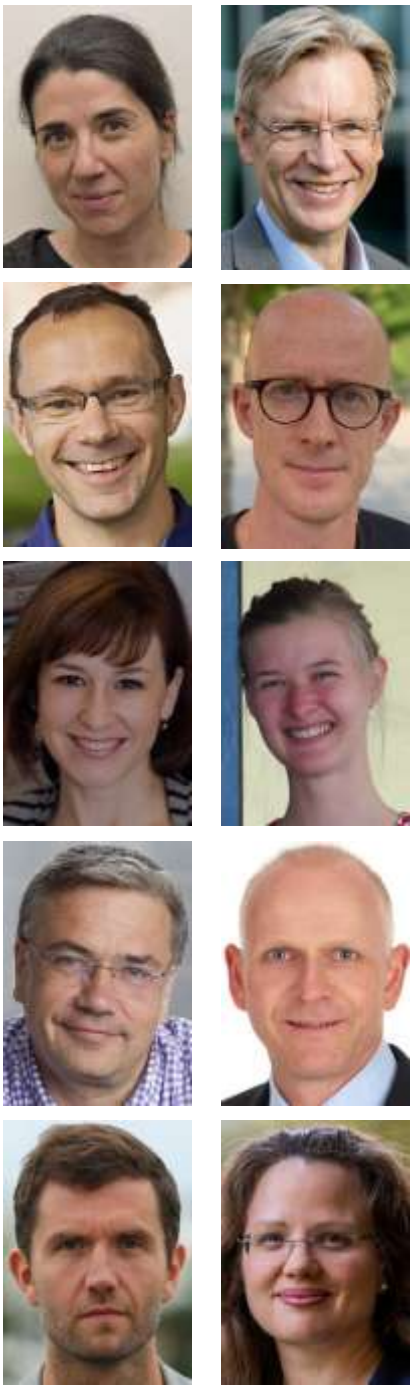
The NordCO$_2$ Steering Committee (SC) met three times during 2020 and twice in 2021, with all meetings being held digitally. The main task of 2020 was the organisation of the Annual and Industry Panel meetings, which were first planned to be held separately in Iceland and Denmark but had to be remodelled to the combined virtual meeting hosted in October. In 2021, the SC worked on the organisation of the Winter School together with the CO$_2$PERATE ITN as well as discussed heavily the planning of the annual meeting for not only 2021, but also the remaining years of the project.

Another central discussion was about the Nordic Exchange Programme, as everyone tried to come up with ideas to stimulate networking and mobility without travelling around. One of these ideas was the organisation of monthly digital seminars, which was agreed on in November 2020. The first seminar of the series was hosted in March 2021, with 8 seminars organised that year.

Amongst the decisions taken by the SC, it was agreed that NordCO$_2$ leader Kathrin H. Hopmann would step down from 2021 due to her duties as the leader of the CO$_2$PERATE ITN, amongst her other activities. NordCO$_2$ co-leader Ainara Nova takes her place, and PI Troels Skrydstrup is stepping up as co-leader until the end of the year. Assoc. Prof. Hopmann remains as NordCO$_2$ PI and representative for UiT in the SC.

It is also our pleasure to have had our midterm evaluation approved by our funding agency NordForsk in 2020, thus securing our funding until the end of the project in 2023.

The aftermath of the COVID-19 pandemic, with its impact on mobility within the consortium, led the SC to redirect some of the unused funds to create a one-year researcher position at UiO. The position is meant to strenghten the participation of UiO in the consortium, where our leader is located. In addition to this, the SC decided to allocate the rest to support the PhD students currently funded by NordCO$_2$.



The NordCO$_2$ Steering Committee

Outlook: Activities in 2022

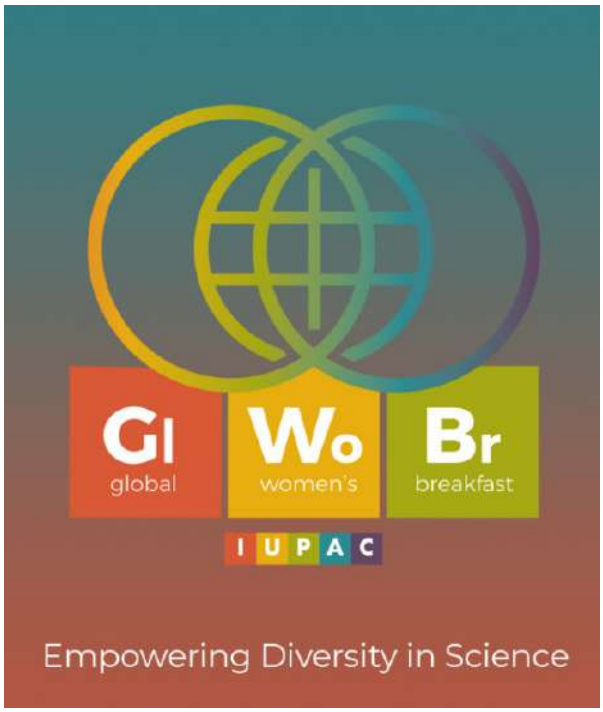
First on the agenda for 2022 is IUPAC's Global Women's breakfast, on the 16th of February. The event is organised each year across the globe and is focused on "Empowering diversity in science". NordCO$_2$ will collaborate with CO$_2$PERATE to organise a hybrid event with a physical breakfast at the participating institutions as well as digital content.

The NordCO$_2$ Monthly Seminar Series will also continue next year, following our success from 2021. Our goal for 2022 is to increase attendance of both NordCO$_2$ members and members of the community at large.

We keep up the hope for 2022, with our Annual Meeting planned as the long-awaited, physical meeting in Iceland. The meeting will take place from the 10th until the 15th of August 2022, near the town of Hveragerði (about 45 km east of Reykjavík). The meeting will include visits to the Blue Lagoon and the Icelandic firm Carbon Recycling.

In addition to Iceland, we will travel once more in 2022 at the occasion of a workshop in Bergen (Norway).

The activities planned for 2022 also include the organisation of the outreach activity "CO$_2$ Day". The concept of the event is to promote our science to the public, usually by the way of participating to outreach events locally at our institutions. The 2020 and 2021 issues were unfortunately cancelled due to the pandemic, but we are looking forward to bringing CO$_2$ chemistry to the public again next year if the conditions allow for it.



Hot springs in Hveragerði near river Varmá and the advertisement for the GBW 2022, with its theme.

Special COVID-19: A slice of life

Faranak Heshmatnia
PhD student (HU)

Here I would like to share a short story of my life during the ongoing COVID-19 pandemic.

I was fortunate to get a PhD position at Helsinki University. I have always dreamed to go to the wonderful city of Helsinki due to its cool people and beautiful islands.

I started my PhD career in March 2020 and was so excited at the prospect of new adventures in Finland. There were however worldwide whispers about the spreading of a new coronavirus called Covid-19…The world was on alert; countries started to impose quarantine regulations and close their borders to countries with a high number of infected patients.

The awful number of devastating news made me sad as well as worried about my flight. There was an unprecedented pressure on me as my country of origin (Iran) was one of the "red spots" at the time. I was however fortunately able to get to Helsinki on the 1st of March 2020.

The next day after my arrival, I had an appointment with my supervisor when he informed me that I had to be in quarantine for almost two weeks due to the regulations. It was a tough time to experience, but I decided to make the most of it and went through some articles related to my project to be more familiar with this new window of my life.

When I was preparing myself to go to the laboratory, the whole country suddenly went into lock down for virtually five months! We were not allowed to go to either the university nor any of the libraries or tourist locations, and shopping centres were closed. It was a frustrating time for me because I did not get the chance to see my colleagues or even communicate with a friend. I felt homesick and can truly say that the pandemic affected me personally in the social and educational aspects.

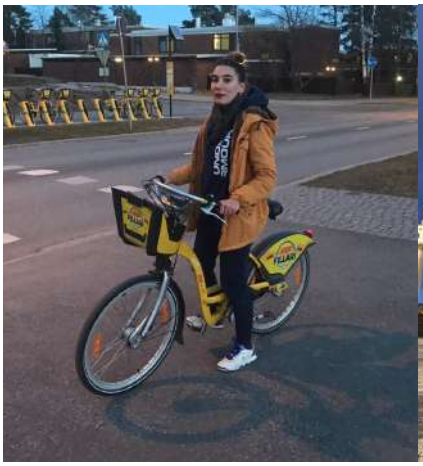
COVID-19 in Iran: Infographic (mefda.ir).

However, we started weekly digital meetings with the whole catalyst group as well as with my supervisor. As I always prefer to communicate face to face, it was great chance for me to get to know the group members and talk about their projects. All the conferences have been either postponed or held digitally and did not fulfil my expectations regarding the quality and output, as it was not as productive as going there physically and have scientific discussions with chemists coming from different universities around the world.

In June and July, we were not allowed to go to the university every day because there was a limit of two people allowed per laboratory at the same time. So, I went to the university three days a week. For experimental research, going to the lab a few days a week means nothing because some experiments take more than three days. I had to find ways to work efficiently in that days. During the summer the girls in the group and I socialized and went to the beach and enjoyed sunshine.

From August, I got the permission to go to the laboratory every day, but office work has not been allowed yet. The situation is better and I started to make friends with the group members. They were so supportive and kind to me which makes this awful Corona time tolerable for me.

In short, it was acceptable to be in quarantine, but it is almost a year that I have been living in Helsinki.
Unfortunately, I have not reached to my goals yet. I feel I am coming down with depression, which makes me worried about my future. Everything has been like a nightmare. On the other side, I am lucky, my loved ones and I are safe and healthy, and I am grateful for all the hardworking during this pandemic.
I wish everyone good health!



From the airport in Iran, and the lone exploration of Helsinki to social activities with the catalyst group (photos: F. Heshmatnia).

Nordic Exchange Programme

The Nordic Exchange Programme (NEP) is the main service provided to the scientific staff within the consortium, allowing research stays of up to six months at any of the institutions participating in NordCO$_2$.

As expected, the travel restrictions of the two last years took a heavy toll on the programme, and only a couple of visits were scheduled, compared to 12 visits in 2019. However, as for meetings, things have been migrating online, and collaborations within the consortium are now happening online, including supervision. This digital mobility has permitted students located at different institutions to not only work on joint manuscripts but also to learn from each other.

The Kröpeliner Tor in Rostock (Germany) during Lichtwoche, the festival of lights held in Rostock in November and December (Photo: J. B. Jakobsen).

AU to LIKAT

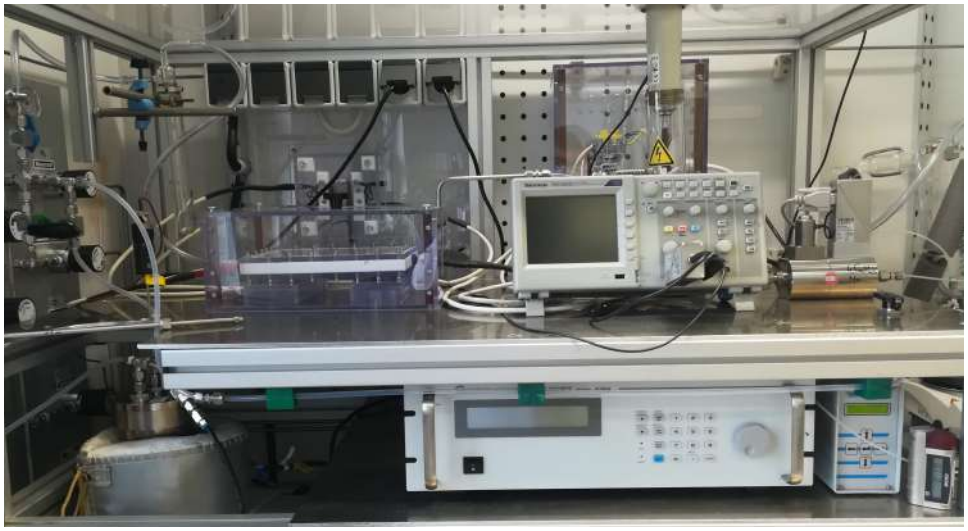
Joakim B. Jakobsen
PhD student (AU)

In the late summer of 2020, I moved to Rostock (Germany) for an exchange stay at the Leibniz-Institut für Katalyse (LIKAT) under the supervision of Prof. Matthias Beller and Dr. Ralf Jackstell. At LIKAT, they recently acquired an experimental plasma-setup, where stable gases such as CO_2 can be activated non-catalytically using high voltage electricity. At the group of Prof. Troels Skrydstrup, I worked with homogeneous electrochemical CO_2 reduction. Therefore, going to Rostock would be an excellent opportunity to get familiar with a different, but still related topic and equipment. At LIKAT, I was tasked to provide proof of principle on the hydrogenation of CO_2 to CO using the plasma-setup. Subsequent work would evolve around the utilization of the produced gaseous products in several reactions. During my stay, I managed to optimize different parameters of both the plasma-setup and the plasma conditions to obtain CO_2 hydrogenation to CO with a high selectivity (minor by-products being CH_4 and MeOH). In the same setup, I also investigated the direct splitting of CO_2 to CO and O_2 and to my delight, this was indeed possible.

Gratifyingly, it was also possible to utilize the produced CO directly in palladium-catalyzed alkoxycarbonylations and rhodium-catalyzed hydroformylations.

Apart from the laboratory work, I had time to visit some of the other group members and enjoy Rostock. In November, I had the pleasure to attend "Die Lichtwoche", which is a tradition in Rostock, where the November darkness is replaced by colorful lights on several of the city's buildings, such as the main building of the University of Rostock and Kröpeliner Tor.

Unfortunately, most attractions in Rostock were closed due to COVID-19, thus, I mainly experienced the city from walks and by glancing through windows. However, I managed to go on several trips to explore the countryside outside of Rostock such as the beautiful sand beach Warnemünde and Germanys largest island Rügen. All in all, I really enjoyed my stay in Rostock and I surely appreciated the opportunity to go physically, in times when it was difficult to travel.



Plasma setup located at LIKAT (Photo: J. B. Jakobsen).

UoI to UiO

Sri Harsha Pulumati
PhD student (UoI)

As a part of the exchange program of the NordCO$_2$ consortium, I had a wonderful opportunity to be a part of a research collaboration between Prof. Egill Skúlason at the University of Iceland and Assoc. Prof. Ainara Nova at the University of Oslo. The collaboration aimed to explore the CO_2 conversion capabilities of Metal encapsulated Metal-organic frameworks. This research allowed me to visit Hylleraas Centre for Quantum Molecular Sciences at the University of Oslo. Oslo is a beautiful city and it was great to interact with the scientific community at the Hylleraas Centre with regular meetings and frequent talks by experts. The collaboration was a great success and over the past year I visited Oslo twice for a month and another much longer visit is on hold due to the pandemic. I cannot wait to return.

The exchange program allowed me to learn about hydrogenation reactions over metal functionalized metal–organic frameworks, Micro kinetic modelling, CP2K code and modelling of reaction mechanisms. I had many interesting discussions with Ainara and Dr. Torstein Fjermestad and learnt many techniques that made my life easier as a computational chemist. I also had the opportunity to learn more about experimental chemistry in various discussions with Prof. Unni Olsbye and her group, this gave me great insights and appreciation for the work I do. I would say this was a great experience and I hope to be part of many more such endeavours.
I strongly suggest my fellow students to take advantage of the exchange program.

A few views that caught Harsha's interest during his stay in Oslo, Norway (photos: S. H. Pulumati).

People

Principal Investigators

Ainara Nova (UiT, UiO)
Associate Professor
Consortium leader

Annette Bayer (UIT)
Professor

Timo Repo (HU)
Professor
leader WP2

Mårten Ahlquist (KTH)
Professor
leader WP3

Vidar R. Jensen (UiB)
Professor
leader WP1

Sascha Ott (UU)
Professor

Troels Skrydstrup (AU)
Professor
leader WP4

Egill Skúlason (UoI)
Professor

Knut Børve (UiB)
Professor

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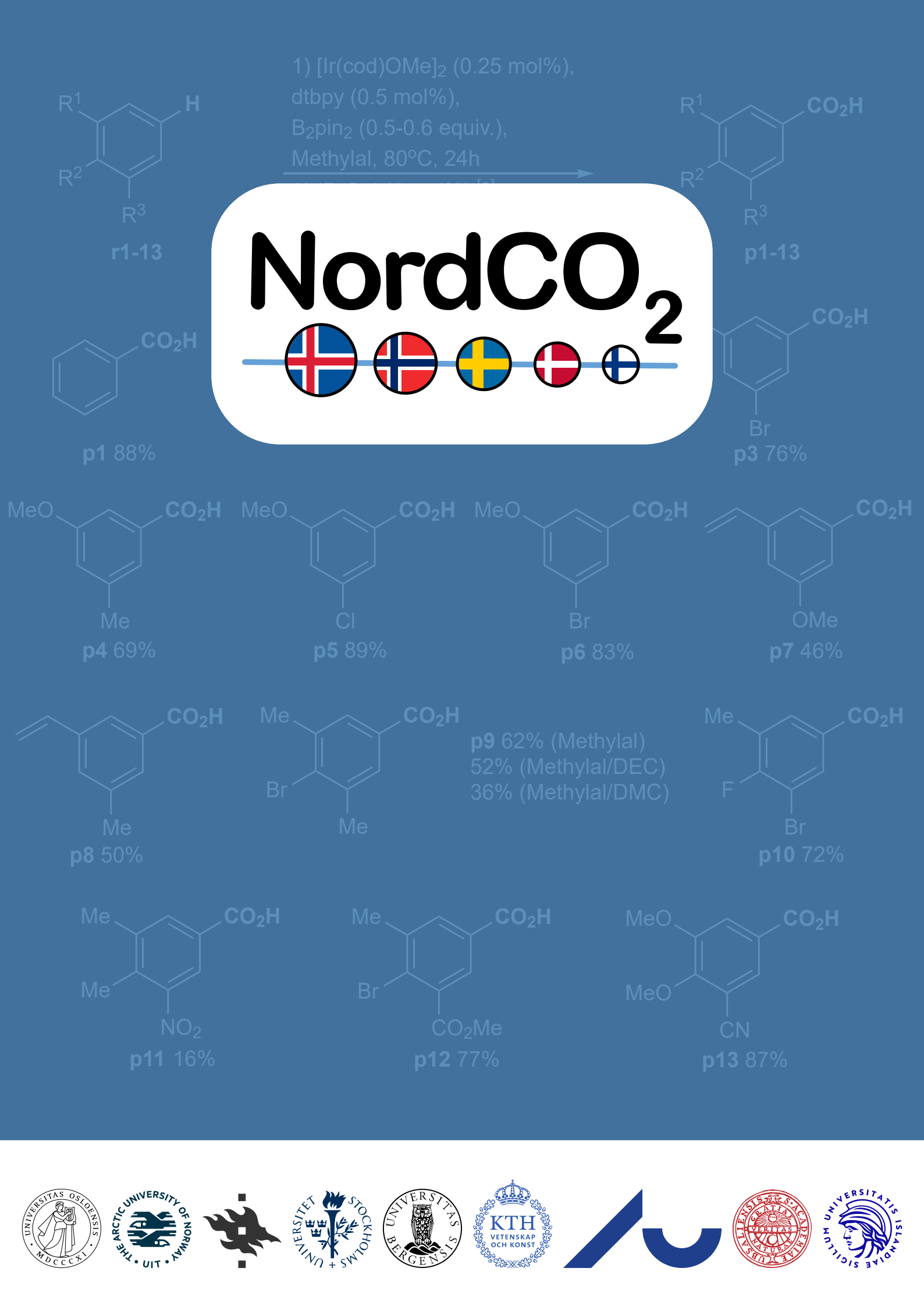
1) [Ir(cod)OMe]2 (0.25 mol%),
dtbpy (0.5 mol%),
B2pin2 (0.5-0.6 equiv.),
Methylal, 80ºC, 24h
r1-13
p1-13
NordCO2
p1 88%
p3 76%
p4 69%
p5 89%
p6 83%
p7 46%
p8 50%
p9 62% (Methylal)
52% (Methylal/DEC)
36% (Methylal/DMC)
p10 72%
p11 16%
p12 77%
p13 87%