NordCO$_2$

The Nordic Consortium for CO_2 Conversion

Annual Report 2018

Cover picture: *Glassware photo from Colourbox/B.Weltmann. The molecular inset shows steps in the conversion of CO_2 to methane from Hussain, Jónsson, Skúlason,* ACS Catal. 2018*, 8, 5240.* ***DOI:*** *10.1021/acscatal.7b03308*

NordCO$_2$ ANNUAL REPORT 2018

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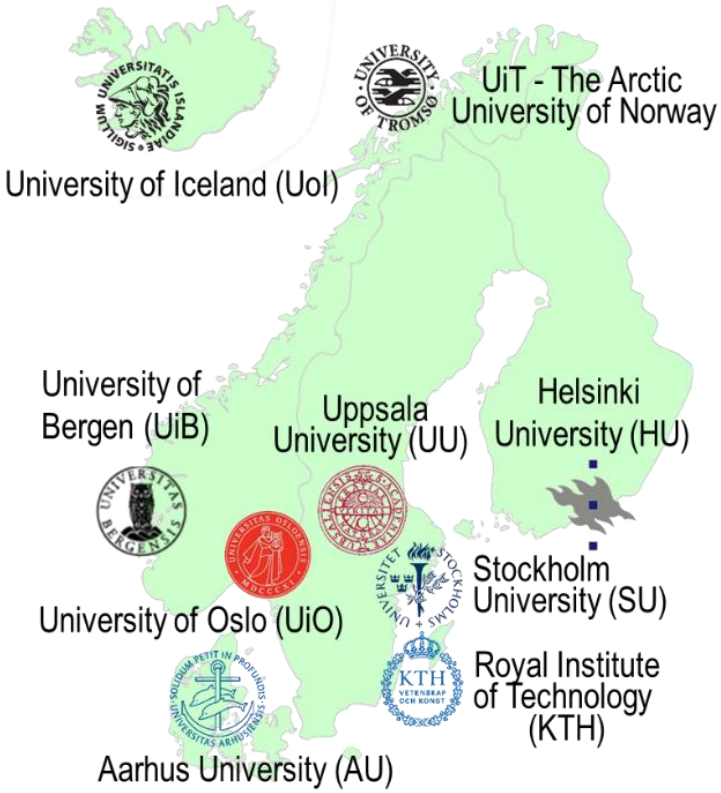

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NordCO$_2$ - OVERVIEW

NORDIC CONSORTIUM FOR CO_2 CONVERSION

The Nordic Consortium for CO_2 Conversion (**NordCO$_2$**) is a Nordic University Hub financed by NordForsk and 9 participating Universities in 5 Nordic countries (Box 1). 13 PIs and their groups are associated with the consortium. The consortium was financed for the years 2018-2020, with an evaluation in 2020. If the evaluation is passed, the consortium will be extended until 2023.

The goal of **NordCO$_2$** is to establish an internationally leading research and training environment on chemical conversion of CO_2 to chemicals and fuels. This is achieved through strengthening the collaborations between excellent Nordic research groups in the field, coupled with meetings, joint courses, summer schools and a Nordic Exchange Program (NEP) for students.

Why are we focusing on CO_2? Many compounds that are indispensable to society, such as fuels, plastics, medicines, and paints (Fig. 1), are currently made from oil. Society will eventually run out of many of these ingredients, which implies that chemical synthesis has to be transformed entirely towards the use of sustainable components. This transformation will take time and effort. A major priority must be given to the development of chemical reactions, which utilize sustainable sources of carbon, the main element in all organic molecules. An example of a sustainable carbon source is carbon dioxide (CO_2), which in photosynthetic processes in Nature is converted to complex organic molecules. **In analogy, CO_2 could become a major carbon feedstock in the academic laboratory and in industrial chemical synthesis.** The use of CO_2 as a carbon synthon is promoted by its many promising features: it is non-toxic, non-flammable, abundant and impossible to deplete.

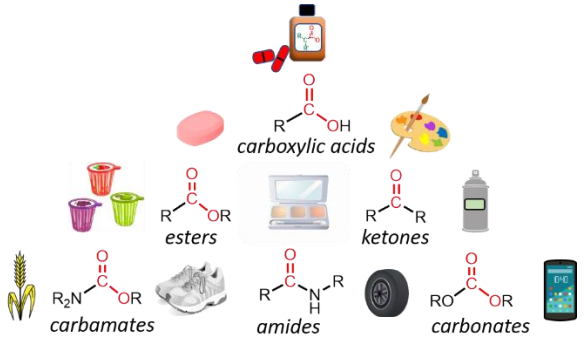


Fig. 1. *Examples of chemicals that are indispensable to our society*

BOX 1: NordCO$_2$ Universities & Funding

NORWAY:
- **UiT – The Arctic University of Norway (UiT)**
  Assoc. Prof. K. Hopmann, Assoc. Prof. A. Bayer
- **University in Oslo (UiO)**
  Dr. A. Nova
- **University of Bergen (UiB)**
  Prof. K. Børve, Prof. V. R. Jensen

SWEDEN:
- **Uppsala University (UU)**
  Prof. S. Ott, Prof. L. Hammarström
- **Stockholm University (SU)**
  Prof. B. Martín-Matute
- **KTH - Royal Institute of Technology (KTH)**
  Assoc. Prof. M. Ahlquist.

DENMARK
- **Aarhus University (AU)**
  Prof. T. Skrydstrup, Prof. K. Daasbjerg

ICELAND:
- **University of Iceland (UoI)**
  Prof. E. Skúlason

FINLAND:
- **Helsinki University (HU)**
  Prof. T. Repo

FUNDING: **NordForsk** (nordforsk.org/en/programmes-and-projects/programmes/nordic-university-hubs) & participating Universities.

NordCO$_2$ - OVERVIEW

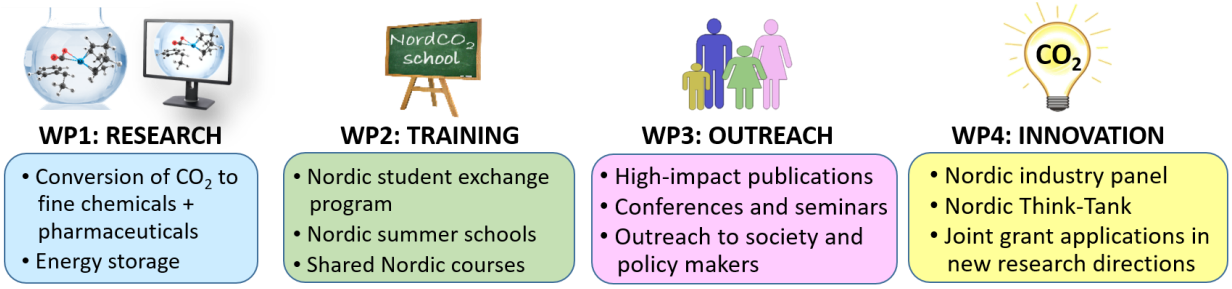


Fig. 2. Work packages in ***NordCO$_2$*** *(picture of empty glassware and PC frame from colourbox.com, C. Kirill)*

NordCO$_2$ comprises computational and experimental chemists working with homogeneous, heterogeneous, electrochemical, and photochemical approaches to develop catalysts for conversion of CO_2 to important chemicals and energy storage molecules such as fuels. The activity in **NordCO$_2$** is overseen by the Steering Committee (SC) with members from all involved Universities and an External Advisory Board (EAB, BOX 2). The **NordCO$_2$** activities are divided into 4 work packages (Fig. 2).

2018 was the first year of the **NordCO$_2$** consortium, during which we have initialized research collaborations and the Nordic Exchange Program, have organized joint courses, and have met at two larger meetings in Norway and Denmark. We have participated in initiation of an open science platform, have organized the outreach activity *Nordic CO$_2$ Days*, have disseminated research results in international journals and have strengthened future collaborations through joint grant applications e.g. to H2020. High-lights from our activities in 2018 and some of the planned activities for 2019 are given in this annual report. We are humbled and excited to continue the **NordCO$_2$** consortium in 2019.

On behalf of the consortium,

BOX 2: NordCO$_2$ SC & EAB

The NordCO$_2$ Steering Committee (SC):
- Kathrin H. Hopmann (Consortium leader, UiT)
- Sascha Ott (WP1 leader, UU)
- Egill Skúlason (WP2 leader, UoI)
- Annette Bayer (WP3 leader, UiT)
- Troels Skrydstrup (WP4 leader, AU)
- Belén Martín-Matute (SU)
- Mårten Ahlquist (KTH)
- Timo Repo (HU)
- Vidar R. Jensen (UiB)
- Ainara Nova (UiO)
- Jere Mannisto (HU, SC student representative)
- Pooria Farahani (KTH, Substitute for SC student representative)

The NordCO$_2$ External Advisory Board (EAB):
- Odile Eisenstein (ICGM, UiO)
- Ómar Freyr Sigurbjörnsson (CRI)
- Ruben Martin (ICIQ)
- Matthias Beller (LIKAT)

Assoc. Prof. Kathrin H. Hopmann
UiT – The Arctic University of Norway
NordCO$_2$ consortium leader
(Photo. D. Jensen/UiT)

Assoc. Prof. Annette Bayer
UiT – The Arctic University of Norway
NordCO$_2$ WP3 leader

NordCO$_2$ - ACTIVITIES

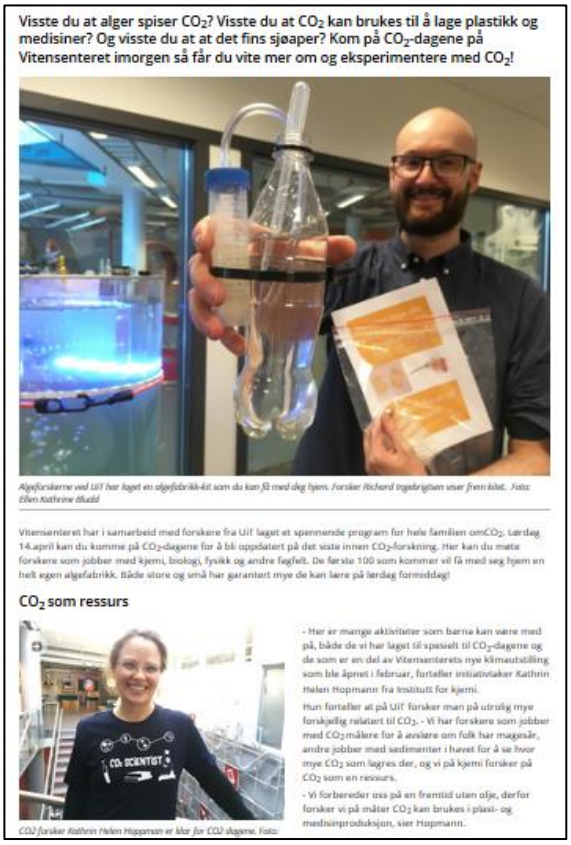
NORDIC CO$_2$ DAYS APRIL 2018

In April 2018, the **NordCO$_2$** consortium helped to arrange the *Nordic CO$_2$ Days* at the Northern Norwegian Science Center. This included various interactive stands with activities and chemical experiments on CO$_2$ in chemistry, in biology, in medicine, in nature, and in food, alongside public science talks and videos on the climate and on ocean acidification. Both PIs and students participated in the preparation of all activities. Several hundred people, including many children, visited the Science centre to play with CO$_2$ and to watch algae eat CO$_2$. As part of the *Nordic CO$_2$ Days*, we made an exhibition on CO$_2$-related research called *Faces of CO$_2$*, which the public could enjoy at the Science Centre from April until September 2018.

Program for the CO$_2$ days.

Left: PhD Student Lj. Pavlovic at the chemistry stand. Right: Video we made for children on the CO$_2$ Days: youtube.com/watch?v=cjd3LG6FGww&feature=youtu.be&fbclid=IwAR3e_ItHkXCqpaLW0KJLjeLUoSfHjI_otoWHdnozRvLlLDmM0TYMEHSkn24

Pictures in the exhibition 'Faces of CO$_2$'.


Visste du at alger spiser CO_2? Visste du at CO_2 kan brukes til å lage plastikk og medisiner? Og visste du at at det fins sjøaper? Kom på CO_2-dagene på Vitensenteret imorgen så får du vite mer om og eksperimentere med CO_2!

Algeforskerne ved UiT har laget en algefabrikk-kit som du kan få med deg hjem. Forsker Richard Ingebrigtsen viser frem kitet. Foto: Ellen Kathrine Bludd

Vitensenteret har i samarbeid med forskere fra UiT laget et spennende program for hele familien omCO$_2$. Lørdag 14.april kan du komme på CO$_2$-dagene for å bli oppdatert på det siste innen CO$_2$-forskning. Her kan du møte forskere som jobber med kjemi, biologi, fysikk og andre fagfelt. De første 100 som kommer vil få med seg hjem en helt egen algefabrikk. Både store og små har garantert mye de kan lære på lørdag formiddag!

CO$_2$ som ressurs

- Her er mange aktiviteter som barna kan være med på, både de vi har laget til spesielt til CO$_2$-dagene og de som er en del av Vitensenterets nye klimautstilling som ble åpnet i februar, forteller initiativtaker Kathrin Helen Hopmann fra Institutt for kjemi.

Hun forteller at på UiT forsker man på utrolig mye forskjellig relatert til CO$_2$. - Vi har forskere som jobber med CO$_2$-målere for å avsløre om folk har magesår, andre jobber med sedimenter i havet for å se hvor mye CO$_2$ som lagres der, og vi på kjemi forsker på CO$_2$ som en ressurs.

- Vi forbereder oss på en fremtid uten olje, derfor forsker vi på måter CO$_2$ kan brukes i plast- og medisinproduksjon, sier Hopmann.

CO2-forsker Kathrin Helen Hoppmann er klar for CO2 dagene. Foto:

Screen-shot of news-item on the CO$_2$ days
(pictures & text by E. K. Bludd/UiT)

NordCO$_2$ - ACTIVITIES

NordCO$_2$ KICK-OFF SYMPOSIUM MAY 2018

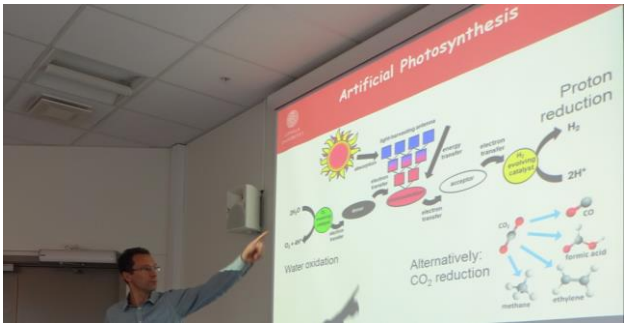
On May 14-16 2018, the **NordCO$_2$** consortium came together for a kick-off meeting at UiT – The Arctic University of Norway. About 35 engaged scientists from Denmark, Sweden, Norway, Iceland, Finland and France gathered at the first **NordCO$_2$** meeting for 2 days of science on CO_2 conversion. The **NordCO$_2$** PIs and members of the external advisory board (EAB) present at the meeting included Egill Skúlason (UoI, Iceland), Ómar Sigbjörnsson (CRI, Iceland), Sascha Ott (UU, Sweden), Kathrin H. Hopmann and Annette Bayer (UiT, Norway), Mårten Ahlquist (KTH, Sweden), Ainara Nova (UiO, Norway), Belén Martín-Matute (SU, Sweden), Odile Eisenstein (ICGM, France), Timo Repo (HU, Finland), Troels Skrydstrup and Kim Daasbjerg (AU, Denmark). The remaining participants were students from the NordCO$_2$ nodes.

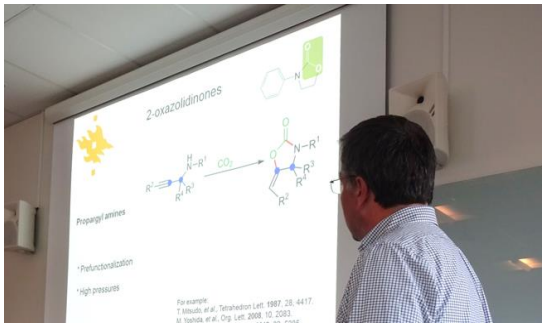
On the 14th, the PIs and the external advisory board (EAB) gathered for dinner to discuss science, collaborations and the meaning of life, accompanied by the marvelous flavors of local cuisine. The 15th started with a Steering committee (SC) meeting, followed by presentations from the PIs and their group members. After the scientific program, the participants dined at the hotel, where Northern specialties were served, such as whale, reindeer and cod. The 15th continued with more opportunities to present chemistry on CO_2 conversion and to discuss collaborations.

After the official part of the program, some participants took the cable car up on Storsteinen (421 m above sea level) for a view of the city of Tromsø (which is located on an island) and the surrounding mountains.

Read more at: site.uit.no/nordco2/2018/05 and site.uit.no/nordco2/2018/04/25/1st-nordco2-meeting

Left: Participants at the first day of the Kick-Off meeting, Right: Breaks allow for discussions between students.





The 2 main topics of NordCO$_2$ include use of CO_2 as an energy storage molecule (here discussed by Sascha Ott, Uppsala University) and conversion of CO_2 to chemicals (here discussed by Timo Repo, Helsinki University)

NordCO$_2$ - ACTIVITIES

NordCO$_2$ COURSES SEPTEMBER 2018

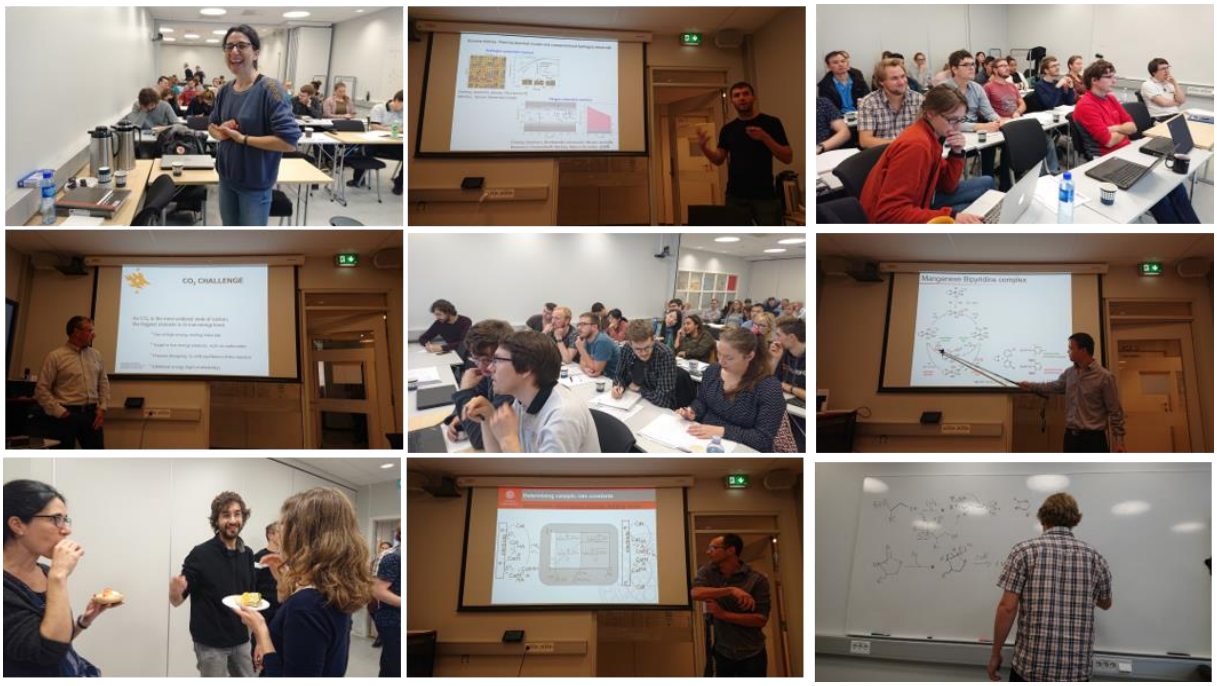
In September 2018, **NordCO$_2$** arranged 2 courses open to **NordCO$_2$** and other interested students: *Python programing for beginners* and *Mechanisms for CO$_2$ activation*

About 30 students participated in the Python course Sept. 4-6, which the HPC group at UiT taught (special thanks to R. Bast and D. Johnson).

Students at the python course.

On September 12-14th, **NordCO$_2$** organized a course on mechanisms for CO_2 activation at UiT, with PIs from the **NordCO$_2$** nodes presenting insights from their own field. About 25 students were attending. The course was open to anyone, but only students within the **NordCO$_2$** consortium received funding for travel and accommodation.

During 3 days, the course covered topics such as thermodynamics and coordination of CO_2, formic acid and methanol synthesis, carboxylations, synthesis of cyclic carbonates and carbamates, carbon monoxide chemistry, heterogeneous CO_2 conversion and experimental and computational techniques to study reaction mechanisms. In between the lectures, the students worked together on challenging exercises. An oral exam was conducted via Skype on October 23rd and 25th, where the students had to present a CO_2 reaction and literature relevant to it. 13 students took the exam, and all passed. The course was rewarded with 4 ECTS.



Impressions from the course 'Mechanisms for CO$_2$ activation'. NordCO$_2$ lecturers included: A. Nova (UiO), T. Repo (HU), E. Skúlason (UoI), T. Skrydstrup (AU), K. Hopmann (UiT), A. Bayer (UiT), X. Hue (AU), & S. Ott (UU). M. Ahlquist (KTH) acted as external sensor on the exam. The course was taken by students from AU, UiB, UiO, KTH, UU, & UiT.

NordCO$_2$ - ACTIVITIES

REFLECTIONS ON THE JOINT CO_2 COURSE

PhD Student Simon S. Pedersen (AU)

The course on *Mechanisms for CO_2 activation* in Tromsø was a very good experience for me and both the location and topic were motivating for me as a young PhD-student. Tromsø is a very beautiful city, and I'd surely like to go there again, and maybe also see the northern lights next time hopefully!

The course itself was indeed interesting as well, since I had not before taken the time to understand and study reactions with CO_2, and this is valuable knowledge in my research group. I was also delighted to see that a lot of the course material involved organometallic reaction mechanisms with CO_2, since this is one of my bigger interests. In addition, I believe the course material and lectures were very well balanced between heterogeneous, homogeneous and theoretical chemistry. I also very much liked the format of the course where exercises were included into the lectures, which helped to keep me focused - even more than the coffee! Thanks for a nice course.

NordCO$_2$ STEERING COMMITTEE MEETINGS

The **NordCO$_2$** Steering committee (SC) met twice during 2018, once at UiT (May) and once at AU (Nov.). All **NordCO$_2$** nodes are represented in the SC, alongside a student representative (see BOX 2, page 3). The SC plans and approves the consortium activities such as the Nordic Exchange Program (NEP), joint courses and summer schools. The members of the external advisory board (EAB) are invited to all SC meetings, but have no voting rights. Between physical meetings, the SC communicates online.

Meeting of the NordCO$_2$ SC at UiT, May 2018

***Left:** Meeting of the NordCO$_2$ Steering Committee at Aarhus University, Nov. 2018. **Right:** At dinner, the SC used the paper table cloth at the restaurant to discuss future scientific ideas.*

NordCO$_2$ - ACTIVITIES

CADIAC MEETING NOVEMBER 2018

The Carbon Dioxide Activation Center (CADIAC) is a Center of Excellence established in 2015 at Aarhus University. CADIAC is funded by the Danish National Research Foundation. Two of the **NordCO$_2$** PIs are part of CADIAC, Prof. T. Skrydstrup, who is the CADIAC director, and Prof. K. Daasbjerg, who is one of the core team leaders at CADIAC. The centre works closely together with two international groups headed by Prof. M. Sanford at the University of Michigan, USA, and Prof. M. Beller at the Leibniz Institute for Catalysis, Germany (who also is part of the External Advisory Board of **NordCO$_2$**). The research at CADIAC focuses on transition metal catalysis for the activation and exploitation of carbon dioxide as a reagent in chemical synthesis.

Every November since 2016, CADIAC has an annual meeting in Aarhus. In November 2018, most of the **NordCO$_2$** PIs attended the CADIAC annual meeting Nov. 19 to 20th at the Marselis Hotel in Aarhus, Denmark, and presented their work. This included A. Bayer (UiT), A. Nova (UiO), T. Repo (HU), E. Skúlason (UoI), M. Ahlquist (KTH), T. Skrydstrup (AU), and K. Hopmann (UiT).

Read more about CADIAC at:
inano.au.dk/about/research-centers/cadiac

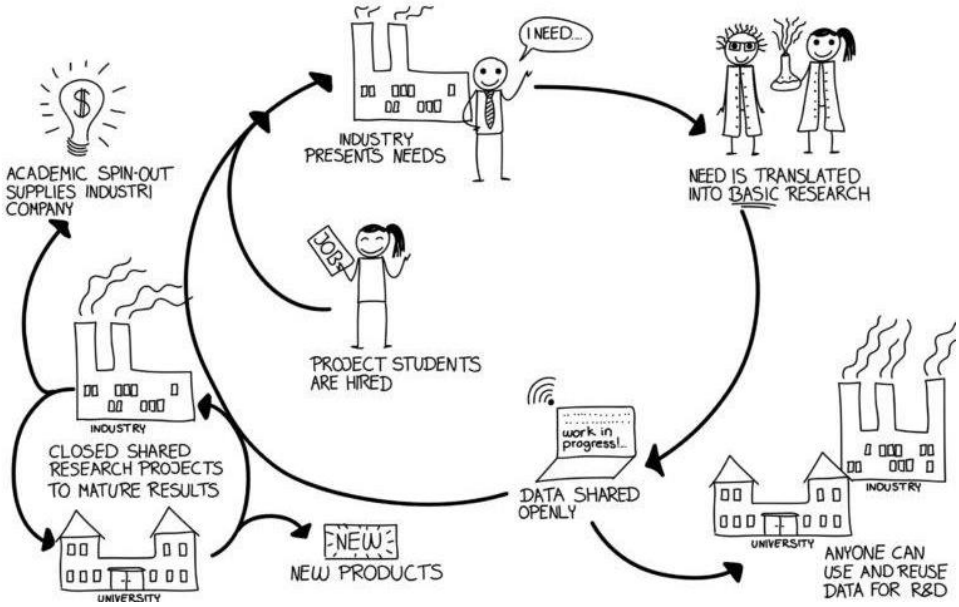
Presentations by NordCO$_2$ PIs A. Bayer (UiT), A. Nova (UiO), T. Repo (HU), E. Skúlason (UoI), M. Ahlquist (KTH) and T. Skrydstrup (AU) at the CADIAC meeting 2018.

NordCO$_2$ - ACTIVITIES

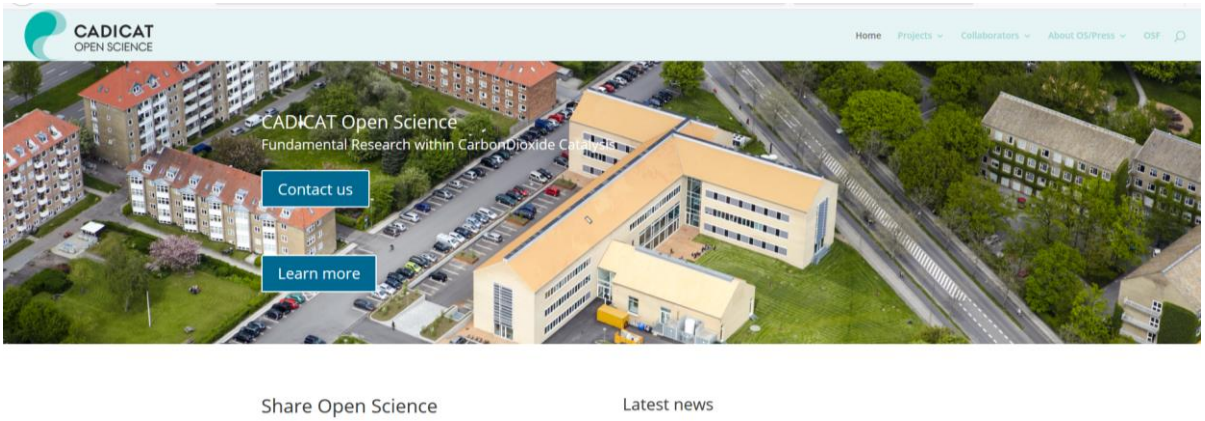
OPEN SCIENCE PLATFORM CADICAT

The **NordCO$_2$** PI K. Daasbjerg at AU has been the initiator behind the open science platform SPOMAN (spoman-os.org), established at AU in 2017 to promote collaborations between academia and industry on polymer materials and nano composites. As SPOMAN was highly successful, this initiative was followed by a new platform opened in 2018 for open science collaborations on CO_2 and Catalysis, named **CADICAT** (cadicat-os.org). On the platform, everyone can present their research and obtain input from academic and industrial partners. The projects are generally open to the entire public, although it is possible to communicate in closed groups. The **NordCO$_2$** consortium is actively supporting the CADICAT platform, and will in March 2019 arrange a course, where all students are trained in using CADICAT for sharing research results and ideas, and for communicating between **NordCO$_2$** nodes.

Read more at: https://cadicat-os.org/about-os/



Concept behind Open Science platforms CADICAT and SPOMAN



Screenshot of the CADICAT platform at https://cadicat-os.org/

NordCO$_2$ - ACTIVITIES

OUTLOOK: NordCO$_2$ ACTIVITIES 2019

For 2019, the **NordCO$_2$** consortium is planning several activities, which include:

MARCH 19 to 20th 2019

A course on **Open Science** will be arranged at KTH in Stockholm, Sweden. The **NordCO$_2$** students will learn how to use the open science platform CADICAT (developed by **NordCO$_2$** PI K. Daasbjerg, AU) and will discuss future scientific collaborations. *Read more about CADICAT at: cadicat-os.org*

JUNE 16 to 20th 2019

NordCO$_2$ PI Prof. Timo Repo (HU) is the main organizer of the **23rd European Conference on Organometallic Chemistry** (EuCOMC 2019) in Helsinki, Finland. This conference covers organometallic chemistry, from fundamental insights to applications in for example catalysis, and it normally features several hundred participants. Several of the **NordCO$_2$** PIs will be presenting at EuCOMC 2019. The **NordCO$_2$** consortium is also sponsoring a parallel track at the conference on chemical CO_2 conversion, which is planned for June 17. *Read more about the conference and register at* helsinki.fi/en/beta/eucomc-xxiii

AUGUST 12 to 16th 2019

NordCO$_2$ will arrange a summer school in Reykjavik, Iceland on *Energy carriers from CO_2* (for example formation of methanol or CO from CO_2). The **NordCO$_2$** PIs will be the lecturers at the summer school, which will be open for students outside NordCO$_2$, provided they have own financing for their trip and accommodation.

*Read more about the summer school and other planned **NordCO$_2$** activities at: site.uit.no/nordco2/activities*

*The 23rd European Conference on Organometallic Chemistry will take place in Helsinki, co-organized and co-sponsored by **NordCO$_2$**. (Picture from: helsinki.fi/en/beta/eucomc-xxiii)*

NordCO$_2$ - RESEARCH

NordCO$_2$ RESEARCH & PUBLICATIONS

The **NordCO$_2$** consortium is composed of Nordic research groups working on chemical conversion of CO_2 to higher-value products such as commodity and specialty chemicals and energy carriers such as fuels. 13 Nordic research groups are currently associated with the consortium, of which 6 groups focus on computational tools and 7 groups focus on experimental approaches to design novel catalysts for CO_2 activation:

The groups of **Prof. Troels Skrydstrup** and **Prof. Kim Daasbjerg** at the CO_2 Activation Centre (CADIAC, Aarhus University, AU) in Denmark work on CO_2 activation through different approaches, including organometallic and electrochemical conversion, read more at: inano.au.dk/about/research-centers/cadiac/

The group of **Prof. Timo Repo** at the University of Helsinki (HU) in Finland works on fixation of CO2 to high value-added chemicals such as carbamates, read more at: helsinki.fi/en/researchgroups/catalysis-and-green-chemistry/research

The groups of **Prof. Knut Børve** and **Prof. Vidar R. Jensen** at the University of Bergen (UiB) in Norway are using computational methods to work on the chemistry of CO_2 activation and fixation, read more at: mn.uio.no/kjemi/english/research/projects/co2-activation-and-fixation/

The group of **Prof. Belén Martín-Matute** at the University of Stockholm (SU) in Sweden is working on catalytic composites for sustainable synthesis, read more at: su.se/english/about/news-and-events/making-chemicals-without-dangerous-intermediate-by-products-1.302979

The group of **Dr. Ainara Nova** at the University of Oslo (UiO) in Norway is working on rational catalyst design for transforming CO_2 into industrially attractive products such as methanol and polycarbonates, read more at: mn.uio.no/kjemi/personer/vit/ainaran

The groups of **Prof. Sascha Ott** and **Prof. Leif Hammarström** at the University of Uppsala (UU) in Sweden work on artificial photosynthesis and CO_2 reduction catalysts, read more at: kemi.uu.se/research/synthetic-molecular-chemistry/research-groups/ott-group and kemi.uu.se/research/physical-chemistry/research-groups/leif-hammarstrom-group

The group of **Assoc. Prof. Mårten Ahlquist** at the Royal Institute of Technology in Sweden (KTH) works on homo- and heterogeneous conversion of CO_2 using diverse computational approaches, read more at: kth.se/profile/ahlqui

Prof. Egill Skúlason's group at the University of Iceland (UoI) works on theoretical studies of heterogeneous catalysts involved in CO_2 conversion, read more at notendur.hi.is//~egillsk/pres.html

The groups of **Assoc. Prof. K. Hopmann** and **Assoc. Prof A. Bayer** at UiT – The Arctic University of Norway (UiT) collaborate on the CHOCO project, which develops homogeneous catalysts for conversion of CO_2, read more at site.uit.no/choco.

In March 2017, the NordCO$_2$ PIs met for the first time at UU to discuss their plans for a Nordic Consortium.

NordCO$_2$ - RESEARCH

The **NordCO$_2$** members regularly publish their research on CO_2 conversion in high-level international journals. Some examples from 2017 and 2018 include:

• **Enantioselective incorporation of CO$_2$: Status and Potential.** J. Vaitla, Y. Guttormsen, J. K. Mannisto, A. Nova, T. Repo, A. Bayer, K. H. Hopmann, *ACS Catal.* 2017, *7*, 7231. DOI: 10.1021/acscatal.7b02306. *Here several NordCO$_2$ PIs (UiT, HU, UiO) jointly provided their view on using CO_2 for making different chiral molecules.*

• **Carbon dioxide-based facile synthesis of cyclic carbamates from amino alcohols** T. Niemi, I. Fernández, B. Steadman, J. K. Mannisto, T. Repo, *Chem. Comm.* 2018, *54*, 3166. DOI: 10.1039/C8CC00636A *The HU group with PI Repo reported a mild and selective method for the synthesis of cyclic carbamates from amino alcohols and CO_2.*

• **Development of a UiO-type thin film electrocatalysis platform with redox-active linkers** B. A. Johnson, A. Bhunia, H. Fei, S. M. Cohen, S. Ott *J. Am. Chem. Soc.* 2018, 140, 2985. **DOI:** 10.1021/jacs.7b13077 *The UU group with PI Ott reported the first conducting MOF thin film platform for future incorporation of molecular catalysts, including for CO_2 reduction. The MOF provides electric conductivity & structural stabilization to the catalyst.*

• **Time-Resolved IR spectroscopy reveals a mechanism with TiO2 as a reversible electron acceptor in a TiO2-Re catalyst CO$_2$ photoreduction system M.** Abdellah, A. M. El-Zohry, L. J. Antila, C. D. Windle, E. Reisner, L. Hammarström, *J. Am. Chem.Soc.* 2017, *139*, 1226. DOI: 10.1021/jacs.6b11308. *The UU group with PI Hammarström explained how TiO_2 enhances the photocatalytic CO_2 reduction rate of a Re(bpy)(CO)$_3$(L) derivative.*

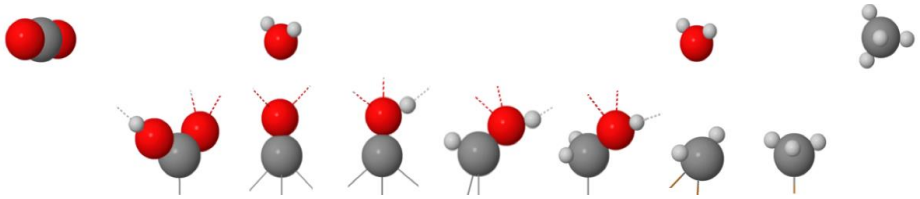
• **Covalently linking CuInS$_2$ quantum dots with a Re catalyst by click reaction for photocatalytic CO$_2$ reduction** J.Huang, M. Gatty, B.Xu, P.B. Pati, A. Etman, L. Tian, J. Sun, L. Hammarström, H. Tian, *Dalton Trans.* 2018, *47*, 10775. DOI: 10.1039/C8DT01631C. *The UU group with PI Hammarström showed by ultra-fast mid-IR spectroscopy that $CuInS_2$ nano-dots decorated with molecular catalysts work for photochemical CO_2 reduction.*

• **The key role of the hemiaminal intermediate in the cron-Catalyzed deaminative hydrogenation of Amides.** L. A. Suarez, Z. Culakova, D. Balcells, W.H. Bernskoetter, O. Eisenstein, K. I. Goldberg, N. Hazari, M. Tilset, N. Ainara, *ACS Catal.* 2018, 8751. DOI: 10.1021/acscatal.8b02184 *Conversion of CO_2 to methanol may occur through different steps, including hydrogenolysis of amides. Here the UiO group with PI Nova investigated the complex iron-catalyzed amide hydrogenolysis.*

• **Carbon-carbon bonds with CO$_2$: Insights from computational studies**, M.Obst, Lj.Pavlovic, K. H. Hopmann *J. Organomet. Chem.* 2018, *864*, 115. DOI:10.1016/j.jorganchem.2018.02.020. *The UiT group with PI Hopmann gave a review how different types of metal catalysts incorporate CO_2.*

• **Mechanistic Studies on NaHCO$_3$ Hydrogenation and HCOOH Dehydrogenation Reactions Catalysed by a Fe^{II} Linear Tetraphosphine Complex.** Marcos, R.; Bertini, F.; Rinkevicius, Z.; Peruzzini, M.; Gonsalvi, L.; Ahlquist, M. S. G. *Chem. Eur. J.* 2018, *24*, 5366, DOI: 10.1002/chem.201704927

• **Selective CO$_2$ reduction to CO in water using earth-abundant metal and nitrogen-doped carbon electrocatalysts** X-M. Hu, ….. M. Beller, S. U. Pedersen, T. Skrydstrup, K. Daasbjerg *ACS Catal.* 2018, *8*, 6255. DOI: 10.1021/acscatal.8b01022



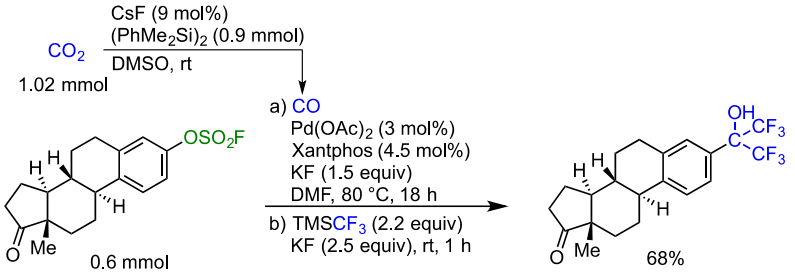
*Steps in the conversion of CO_2 to methane on a Cu(111) surface (not shown), from **Calculations of product selectivity in electrochemical CO$_2$ Reduction** J. Hussain, H. Jónsson, E. Skúlason,* ACS Catal. *2018, 8, 5240. **DOI:** 10.10 21/acscatal.7b03308*

NordCO$_2$ - RESEARCH

RESEARCH HIGHLIGHT FROM AU:
New Chemical Transformations via CO

Organofluorine compounds are well represented as pharmaceuticals and agrochemicals, as the introduction of a fluorine atom can strategically alter the chemical and biological properties of such bioactive compounds. Over the last few years, an increasing number of fluorine-containing drugs have been launched, justifying the need for new synthetic methodologies centered on the incorporation of fluorine-containing motifs. One of these privileged motifs is the bis(trifluoromethyl)carbinol group (see figure). Compounds containing this substructure have shown biological activity against cancer, diabetes, hepatitis C, dyslipidemia and inflammation (Scheme 1a). An interesting feature of the bis(trifluoromethyl)carbinol motif is the presence of a large number of fluorine atoms, which renders them as promising contrast agents for ^{19}F-MRI. We reported in *Angewandte Chemie International Edition* on an efficient procedure for the direct formation of (hetero)aryl bis(trifluoromethyl)carbinols from the corresponding (hetero)aryl bromides and fluorosulfates. This method relies on a Pd-mediated carbonylation with stoichiometric amounts of carbon monoxide and trifluoromethyltrimethylsilane. Particularly noteworthy with this protocol is its ease in operation, but also its suitability even in the presence of a wide range of other functional groups. We were also able to demonstrate that this transformation could be coupled up to a selective CO_2-to-CO reduction. This chemistry will undoubtedly allow for the rapid introduction of the bis(trifluoromethyl)carbinol unit into a wide variety of pharmaceutically relevant molecules.

Reference: *Direct Access to Aryl Bis(trifluoromethyl)carbinols from Aryl Bromides and Fluorosulfates via a Pd-Mediated Carbonylation,* K. Domino, C. Veryser, B. A. Wahlqvist, C. Gaardbo, K. T. Neumann, K. Daasbjerg, W. M. De Borggraeve and T. Skrydstrup, *Angew. Chem. Int. Ed.* **2018**, *57*, 6858.



A direct route to (hetero)aryl bis(trifluoromethyl)carbinols from the corresponding bromides and fluorosulfates.

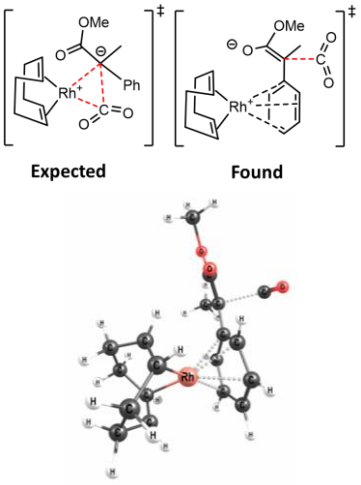
NordCO$_2$ members that participated in this research include K. Domino, K. T. Neumann, K. Daasbjerg and T. Skrydstrup from the CADIAC centre at AU (read more at: inano.au.dk/about/research-centers/cadiac).

NordCO$_2$ - RESEARCH

RESEARCH HIGHLIGHT FROM UiT:
How does CO_2 form Carbon-Carbon bonds?

The **CHOCO** group (site.uit.no/choco) is located at the Northern-most University in the world, UiT – The Arctic University of Norway. The group uses computational and experimental methods to investigate and design novel catalysts for conversion of CO_2. The **CHOCO** project is funded by a 4-year recruitment grant from the Tromsø Research Foundation (tfstiftelse.no). In 2018, the group has focused its research on understanding the mechanistic details of carbon-carbon bond formation with CO_2. A computational analysis by PhD student Ljiljana Pavlovic (*Organometallics* **2018**, *37*, 941) of a known rhodium catalyst (*Eur. J. Org. Chem.* **2016**, 3166) showed that C-C bond formation occurs through an unusual transition state, where the metal catalyst is not interacting with the CO_2 molecule or with the nucleophilic carbon that forms a bond to CO_2 (see figure). This insight is relevant to design catalytic systems that provide better activation of CO_2, which is an inert molecule.

Currently the group is extending its work to other metals. **CHOCO** PhD student Marc Obst and postdoc Ashot Gevorgyan are using computational and experimental techniques to analyze C-CO_2 bond formation catalyzed by copper-catalysts developed in the group of **NordCO$_2$** PI Prof. Skrydstrup (AU). **CHOCO** Postdoc Diego Garcia-Lopez is investigating C-CO_2 bond formation catalyzed by nickel-complexes, using high-level computational methods, which take into account both dynamic effects and solvation, in collaboration with the group of **NordCO$_2$** PI Ainara Nova (UiO).



Computational model of the optimized transition state for C-CO_2 bond formation with a Rh-catalyst, for details see reference below.

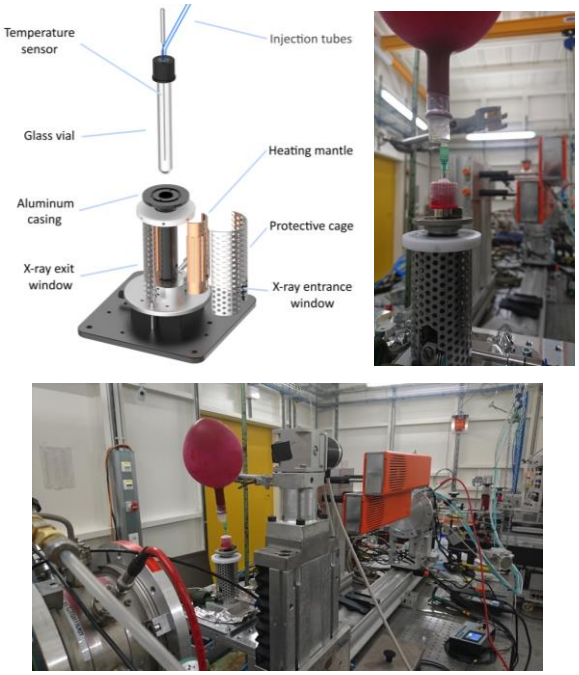
Reference: *Rhodium-Catalyzed Hydrocarboxylation: Mechanistic Analysis Reveals Unusual Transition State for Carbon–Carbon Bond Formation* Lj. Pavlovic, J. Vaitla, A. Bayer, K. H. Hopmann. *Organometallics* **2018**, *37*, 941. DOI: 10.1021/acs.organomet.7b00899

NordCO$_2$ members that participated in this research include Lj. Pavlovic, M. Obst, J. Vaitla, A. Gevorgyan, D. Garcia Lopez, A. Bayer and K. Hopmann in the CHOCO group at UiT (read more at site.uit.no/choco).

NordCO$_2$ - RESEARCH

RESEARCH HIGHLIGHT FROM SU: Heterogeneous Carbonylation Catalysts

The group of Prof. Martín-Matute at SU is currently working on the synthesis of catalytic composites able to reduce CO_2 electrochemically, and use the *in-situ* generated CO in Pd-catalyzed carbonylation reactions. Presently, they are studying the mechanism of the carbonylation reaction using X-ray Absorption Spectroscopy (XAS). They have recently published an article showing the potential of a designed cell for operando XAS studies of organometallic reactions under heterogeneous conditions (*JACS* **2018**, *140*, 8206). Further, the group is also working on the synthesis of oxoalkylcarbamates from CO_2, amines and enols or enol derivatives through an unprecedented reaction that involves a reactivity umpolung of the enol/enol derivatives (work in progress). In addition, the group is working on the synthesis of cyclic carbonates using heterogeneous catalysts based on metal-organic frameworks (MOFs) (work in progress and Perspective submitted for publication).

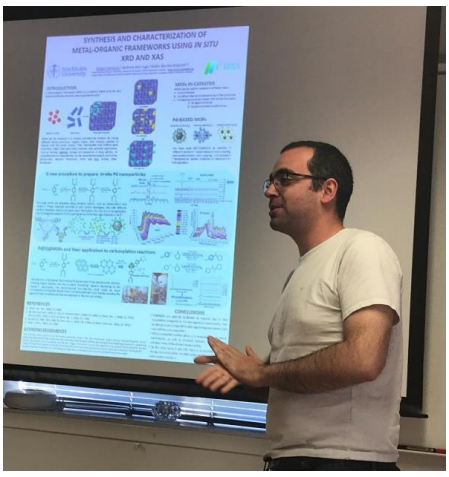


Experiments at Beamline P64, PETRA III, Martín-Matute group (Schematic picture from Yuan et al. 2018, see full ref. below).

Relevant References:

• *Probing the Evolution of Palladium Species in Pd@MOF Catalysts during the Heck Coupling Reaction: An Operando X-ray Absorption Spectroscopy Study* N. Yuan, V. Pascanu, Z. Huang, A. Valiente, N. Heidenreich, S. Leubner, A. K. Inge, J. Gaar, N. Stock, I. Persson, B. Martin-Matute, X. Zou, *J. Am. Chem. Soc.* **2018**, *140*, 8206. DOI: 110.1021/jacs.8b03505

• *Versatile Heterogeneous Palladium Catalysts for Diverse Carbonylation Reactions under Atmospheric CO Pressure* M. Vico Solano, G. González Miera, V. Pascanu, A. K. Inge, B. Martín-Matute *ChemCatChem* **2018**, *10*, 1089. DOI: 10.1002/cctc.201701439



***NordCO$_2$** Postdoc at SU Sergio Carrasco is presenting recent results.*

NordCO$_2$ members participating in this research are S. Carrasco, A. Sanz-Marco, B. Martín-Matute.

NordCO$_2$ - RESEARCH

OVERVIEW NORDIC EXCHANGE PROGRAM

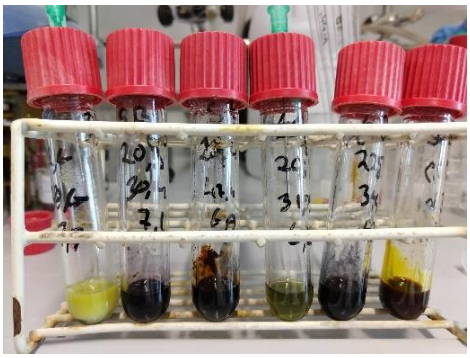
NordCO$_2$ PIs are collaborating through a Nordic Exchange Program (NEP), where all groups send and host students from the consortium. The research visits are minimum 2 weeks and can last several months. In 2018, in addition to the other activities in the consortium, we had 4 NEP visits, which were from HU to AU and UU and from UiT to SU and HU. Two of the visits are described below.

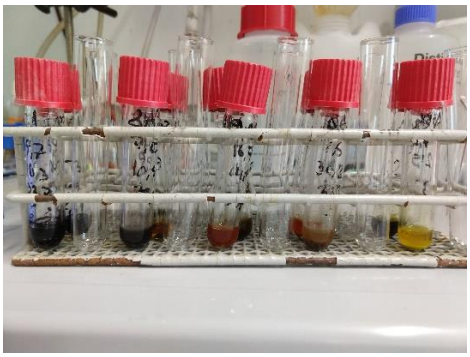
NORDIC EXCHANGE PROGRAM: HU TO AU

PhD Student
Aleksi Sahari (HU)

During the first NordCO2 meeting in May 2018 in Tromsø, my supervisor Prof. Timo Repo (HU) and me were talking with Prof. Troels Skrydstrup (AU). Together we realized that we have related projects focusing on reductive carbon – carbon bond formation with CO_2 with transition metal catalysts. To start a collaboration, I decided to visit the group of Prof. Skrydstrup in Aarhus for three weeks. When I arrived at the laboratories and got to talk with the students, I realized many of them have very in-depth knowledge about nickel chemistry. My background has been mainly in metal-free and copper chemistry and therefore I tried to absorb as much as I could.

We decided that I should join a project working on CO_2 coupling to aldehydes, which was at an idea level at that point. The idea was to use reductive nickel catalysis to generate a nucleophilic carbon on the aldehyde, which could react with CO_2. My task during the visit was to screen a variety of conditions (solvent, ligand, temperature and additives) for the reaction to see if it was possible. The screening was performed in COware tubes (screw cap pressure tubes), which was new for me. The tubes allowed quick injection of CO_2 with a needle to the reaction mixture, which was convenient in contrast to Schlenk tubes and non-screwcap pressure tubes and this saved quite a bit of time. I was happy to see that up to 12 reactions could be set up per day due to the convenient equipment. Unfortunately, even after an extensive screen, no hits were found and side reactions seemed to dominate. Despite this, the trip was definitely not wasted as I learned a lot, got a new scientific ideas and got to enjoy the city of Aarhus.





NordCO$_2$ - RESEARCH

NORDIC EXCHANGE PROGRAM: UIT TO HU

PhD Student

Ljiljana Pavlovic (UiT)

I visited the group of Prof. Timo Repo at the University of Helsinki (HU) from 24th of Nov. to the 8th of Dec. I experienced two beautiful weeks there. Helsinki is a wonderful city with beautiful churches, architecture and museums, and it made me realise I have to come back.

The main goal of my visit was to get insights into the chemistry that Prof. Repo's group is doing in the laboratory and then to apply that in the study of the reaction mechanisms using computational methods. At the Kumpula campus, where the Dept. of Chemistry is located, I enjoyed working with Jere and Jussi, who are both great organic chemists. They shared their experiences with me and we discussed a lot about chemistry. Currently, they are working on a chiral guanidine, which they plan to use as a catalyst in an asymmetric Michael addition. One of the substrates in this reaction is cyclic carbamate, which is synthetized from CO_2. During my stay, I computed a few achiral guanidine catalysts and we are now planning to expand this study to asymmetric reactions.

Presently, in our group, we are working on enantioselective CO_2 conversion into carboxylic acids using bidentate chiral ligands. This trip gave me an opportunity to expand my knowledge on asymmetric reactions and Brønsted base catalysis. As a computational chemist, I do not spend much time in the laboratory, however at HU, I had a chance to observe experiments involving CO_2 chemistry, and it was a really nice experience.

Special thanks to Jere and Prof. Repo for making my visit educational and fascinating.

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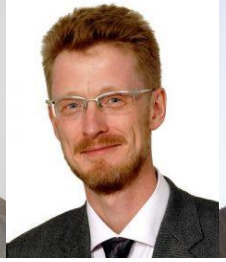

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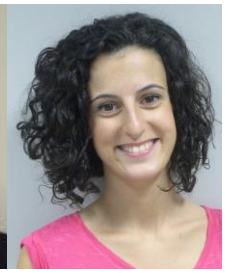

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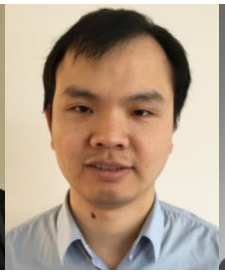

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