For annonsen (max 1500 tegn)

Metal-based catalysts for conversion of CO2

Increasing atmospheric CO_2 is a major concern due to its link to climate changes. On the other hand, CO_2 is an abundant, relatively non-toxic and cheap feedstock of carbon and the ultimate carbon source for a CO_2-neutral economy. As of today, efficient recycling of CO_2 into high-value products like fuels (e. g. methanol, formic acid) or fine chemicals (e.g. organic carbonates, carboxylic acids) is limited by the lack of efficient catalysts.

The research team led by Dr. Kathrin H. Hopmann (theoretical chemistry) and Dr. Annette Bayer (organometallic/organic chemistry) aims to develop novel metal-based catalysts for transformations of CO_2 (see also site.uit.no/choco). To reach this goal, the team employs a combination of computational and experimental approaches. The prospective candidate will work on computational studies of metal-based catalysts, with the goal to obtain a detailed understanding of factors relevant for catalyst performance. The insights obtained will be employed to design novel catalysts. Relevant candidates for the position should have a background in computational chemistry, preferably with experience in organometallic applications.

Catalyst design for sustainable catalysis

Background

Catalytic processes are of economic importance as they reduce the consumption of energy and raw material of chemical reactions. It is assumed that over 90% of chemical products rely on a catalytic step during their production. Transition metal catalyzed homogeneous reactions are important research areas within academia and industry, with a number of industrial processes in use today, e.g. the palladium-catalyzed carbonylation toward the anti-inflammatory Ibuprofen (Boots-Hoechst-Celanese) or the iridium-catalyzed reduction in the production of the herbicide Metolachlor (Ciba-Geigy). The waste majority of catalysts employed in homogeneous reactions are based on precious metals (e.g. Ir, Ru, Pd). However, precious metals are a limited resource and there is a trend in catalyst development to move towards earth-abundant, more environmental-friendly, non-precious metals (e.g. Cu, Fe, Co). Important advances in non-precious metal catalysis have been reported during the last decade, but there is a need for improved catalysts as well as new catalysts for transformations like C-H activation and CO_2-modification. To guide catalyst development, a profound understanding of the mechanistic aspects of non-precious metal catalysis is needed.

Project and approaches

The project is associated with the research team of Dr. Kathrin H. Hopmann (theoretical chemistry) and Dr. Annette Bayer (organometallic/organic chemistry). The team is combining computational and experimental studies to understand and improve metal-based catalysts and to develop novel systems based on non-precious metals. The candidate will be associated with the newly funded CHOCO project (site.uit.no/choco). Key components of the project are:

- Computational studies of catalytic processes for CO_2 modification, with the goal to elucidate mechanistic aspects determining reactivity and stereoselectivity.
- Design of novel ligands and catalysts based on the mechanistic understanding.
- Close interaction with experimentalists for synthesis of relevant systems, identification of reaction intermediates and analysis of reactivity (TON, TOF) and selectivity.

Two postdoctoral researchers and one PhD student are currently associated with the project, with several additional positions being in the process of hiring. Candidates with background in computational chemistry, but with a keen interest in practical applications, are welcome.

Future strategies

Future topics that are relevant to the project are C-H activation in combination with CO_2-modification, where the focus will be on the development of non-precious metal catalysts for fine chemical production.

Research environment

The project will be associated with the theoretical chemistry (TCG) and the organic chemistry (OCG) groups at the Dept. of Chemistry, UiT. The TCG has ~24 members (2 profs., 1 assoc.prof., 3 researchers) and is part of a Centre of Excellence in Theoretical and Computational Chemistry (www.CTCC.no). The TCG has access to advanced super computer facilities through NOTUR.

The OCG has 5 PIs (2 profs., 2 assoc.prof., 1 researcher), thereof 3 working in fields relevant to this project. The OCG is well equipped with instrumentation relevant for the project (e.g. NMR, glovebox, HRMS) and has access to complementary equipment at the Barents Biocentre Lab.

The research environment is highly international. The successful candidates will receive close guidance and support, including participation in the AURORA program for early career development and mentorship of outstanding researchers.