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. Hopman (theoretical chemistry) and Dr. Annette Bayer (organometallic/organic chemistry). The team is combining computational and experimental studies to understand and improve metal-based catalysts. The candidate will be associated with the newly funded CHOCO project (site.uit.no/choco). Key components of the project are:

- Explore new reactivity involving CO_2 as a carbon source by screening of catalyst.
- Experimental studies of the most promising candidates from *in silico* studies of own and known catalytic systems with focus on reactivity (TON, TOF) and selectivity.
- Spectroscopic identify of organometallic intermediates to support the *in silico* proposals.

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 organic or organometallic chemistry and good knowledge in development of metal catalyst 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 an RCN-funded 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. Successful MSCA candidates will receive close guidance and support, including participation in the AURORA program for early career development and mentorship of outstanding researchers.