

ORGANIC CHEMISTRY AND CATALYSIS (OCC)



For master students within the Nanomaterials Science program, the Organic Chemistry and Catalysis (OCC) group offers the opportunity to take part in a specialized research project in the fields of organic and organometallic chemistry, green chemistry and homogeneous catalysis. The group offers a stimulating and dynamic research environment at the forefront of chemical

sciences and chemical synthesis in particular, in an internationally oriented research team.

The synthesis of chemical building blocks and new organic compounds with interesting physical, biological, or pharmaceutical properties remains as a challenge for chemists. Recent and ongoing developments specifically ask for 'clean' and efficient synthesis protocols, preferably based on renewable resources, to be developed for current and future applications. Catalysis plays an important role in the development of such 'clean' and sustainable synthetic protocols.

Within the OCC group, research is done at the interface of organic and inorganic chemistry, including the design of homogeneous, heterogeneous or hybrid catalyst systems that can be used in organic synthesis or the utilisation of renewable feedstocks, such as biomass and CO₂. In homogeneous catalysis, the unique properties of ligand-bound transition metal ions are used to activate substrates and mediate new bond-forming or bond-breaking processes in a highly selective manner. The OCC group chooses to work mainly with first-row transition metals such as Fe, Co, Ni, Cu and Zn as these are more earth-abundant and are generally considered more sustainable. Ligand design is a very important factor for directing the activity and selectivity of a catalyst. In the OCC group, ligand designs vary a lot in terms of composition, structure, bulkiness and denticity. Some ligands bind to a single metal ion, while others bind to two metal ions and can promote unique metal-metal interactions. In addition, new concepts in ligand design are pursued, e.g. through the development of cooperative "non-innocent" ligands, dinucleating ligands, and the design of ligands based on less traditional donor atoms like Si. Research involving heterogeneous and hybrid catalysts, focuses on the utilisation and valorisation of renewable feedstocks such as lignin and CO₂. These processes are supported by numerous industrial partners that contribute to the diversity and applicability of the OCC's academic research. A final research direction in the group is evaluating the viability of green processes through life cycle assessments.

Ongoing research themes:

- New organometallic catalysts derived from first-row transition metals, e.g. Fe, Ni, Cu.
- The development of "non-innocent" ligands that cooperate with a metal centre during catalytic reactions.
- Making bioinspired synthetic complexes that model metalloenzyme active sites, and testing their reactivity in oxidation catalysis.
- Design and synthesis of bimetallic catalysts for sustainable chemical transformations.
- The utilisation of lignin through homogenous and heterogeneous catalysis for a circular chemical industry.
- Development of novel materials for CO₂ capture and conversion to chemical building blocks.

The OCC group hosts most of the required instrumentation and equipment for its research within its own laboratories. The group offers extensive facilities for the synthesis, handling and characterisation of reactive organometallic compounds. Some of the most commonly used techniques for the characterisation of (paramagnetic) organometallic complexes include NMR (multi-nuclear), EPR, ESI-MS, UV-Vis, IR, CV, GC, GC/MS, and HPLC. For single crystal X-ray crystallography, a close collaboration exists with the Crystal & Structural Chemistry group of the Bijvoet Institute. For the (spectroscopic) characterization and application of solid materials, the group closely collaborates with the Inorganic Chemistry & Catalysis (ICC) group. Whereas most research projects are largely comprised of synthetic experimental work and catalyst testing, quantum-mechanical calculations are often used in both the design and interpretation parts of the projects.

COLLABORATIONS AND INTERNSHIPS

Coordinator: Dr. ing. D.L.J. Broere

Staff: prof. dr. Bert Klein Gebbink, prof. dr. Pieter Bruijninx, dr. Marc-Etienne Moret, dr. ing. Danny Broere

Students carry out a research project under the supervision of one of the PhD students or postdocs of the group. They learn to apply the techniques to do catalysis and those that are required to make and handle organometallic compounds and organic reagents in a safe manner. Depending on the topic of the project, the student will investigate synthetic aspects of the development of ligands and (often air-sensitive) organometallic transition metal complexes, and investigate the use of such metal complexes in catalysis, which may amongst other include kinetic analysis and substrate scope studies. Projects can also deal with the development and characterization of molecularly-defined solid catalysts and their application in chemical building block synthesis. Identification and characterization of new ligands, complexes and materials is carried by the students themselves and may include a multitude of different spectroscopic and physico-chemical techniques.

REQUIREMENTS

Recommended bachelor courses: Organic Chemistry (BSc, year 2:SK-BORC13 and 3:SK-BORC3); Organometallic Chemistry (BSc, year 3: SK-B3OMC); Catalysis (BSc, year 3; SK-BKATA);

Recommended Mandatory and primary elective courses: Advanced Organic Synthesis (SK-MOSS); Organometallic Chemistry and Homogeneous Catalysis (SK-MOCHC).

FOR MORE DETAILS CONTACT

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