LABORATORY FOR CHEMICAL TECHNOLOGY
Technologiepark 125, 9052 Gent, Belgium

Supervisor(s)	Period	Funding
Prof. Mark Saeys	4 years	COBICAT

Full-time, funded PhD position: Computational catalyst design for biomass conversion to sustainable aviation fuels

Aim

First-principles modelling-guided design of heterogeneous catalysts to convert biomass-derived small molecules to long-chain sustainable aviation fuel precursors.

Justification

The aviation sector contributes 14% of the CO_2 emissions associated with transport in Europe, yet, it will continue to rely on energy-dense liquid fuels for the foreseeable future. It is hence imperative to develop sustainable alternatives. In this project, we aim to develop an innovative flow process that combines heterogeneous and electrocatalysis for the conversion of aqueous bio-alcohols into aviation fuels.
Process-modelling has shown that this low-temperature liquid phase route and the inherent separation of the fuel precursor from the aqueous phase offer significant benefits over alternative high temperature routes when it comes to the need for separation and CAPEX-intensive H_2 production.
In this project, we will focus on studying the ***thermo-catalytic step*** in liquid phase. The multifunctional catalyst must meet specific criteria to selectively produce long-chain precursors, taking into account factors such as the nature of different active sites and the catalyst's porosity.
We will develop and test bifunctional heterogeneous catalysts which combine a metal active site with acid or base sites. Within the COBICAT project, several types of catalysts will be synthesized and tested using model reactants in an efficient small-scale batch reactor by another PhD student in the team (already started).
The design of the multifunctional catalyst and the optimization of the reaction conditions will be guided by computational catalysis.
Your role in your PhD research will be to tackle the ***computational catalysis*** part of the project. You will investigate appropriate catalyst structures and support the characterization efforts of your colleague through quantum chemical simulations.
Your work will start from an ongoing thesis project that explores appropriate computational methodologies for investigating different catalysts. Several levels of theory will likely be needed, depending on the research question, and you will build expertise on advanced computational catalysis methods.

Program and job description

- Under the supervision of a professor and a postdoc researcher in the team, you will prepare a PhD dissertation over a duration of about 4 years. In these 4 years you publish and present results both at international conferences and in scientific journals.
- You will investigate structure-reactivity relationships for the thermocatalytic condensation reaction using advanced computational catalysis tools.
- You will support the interpretation of experimental results obtained by your project colleagues at UGent.
- You will assist the research group with limited educational tasks in topics related to your research.

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Advisor

- Prof. Mark Saeys

Funding

COBICAT

Candidate Profile

Requirements

- Holder of a Master degree in Chemistry, Chemical Engineering, or equivalent.
- A strong interest in catalysis and motivation for computational catalysis
- A good understanding of physical chemistry on the molecular level
- Experience with computational chemistry is a plus
- Experience with kinetic modeling is a plus.
- You work independently and have a strong feeling of responsibility for your project.
- A good proficiency in English (oral and written)

How to apply and application process

Apply before 1 April 2024 by sending an email to vacatures.saeys@ugent.be. Your application should include:

- your resume (curriculum vitae)
- motivation letter
- a copy of your diploma and diploma supplement (with overview of all courses followed)

Qualified candidates will be invited for an interview as applications are evaluated. In the interview the candidate is expected
This PhD position is available immediately and is open until the vacancy is filled.
More information: mark.saeys@ugent.be

A Ph.D. at UGent and the LCT

We offer a challenging, stimulating, young and pleasant research environment where you can contribute to solving real-life problems for technological innovations with a clear societal as well as economic value. The UGent doctoral school program offers possibilities for following a range of courses or trainings of your interest. We foresee a competitive remuneration and the possibility to obtain a PhD degree in Engineering. You will receive a PhD scholarship for 4 years, with an evaluation after the first year (1+3 contract).

The PhD position offers a unique opportunity to dedicate yourself to fundamental research questions in catalysis in an applied, industrially relevant, and collaborative framework. Your workplace (LCT) is an international environment with intense contacts with industry, and with professionally engineered and operated experimental facilities. The LCT is embedded in the University of Ghent, a world-renowned research university. The Saeys research group is focused on catalysis and technologies for CO_2 conversion with expertise in modelling-guided catalyst design coupled to experimental kinetic validation and state-of-the-art characterization. The lab offers opportunities to guide master students and to support education.
The offer includes:

- A 100% PhD Scholarship (1+3, coupled with a positive evaluation after Y1).
- Full-time employment with 36 days of holiday leave per year.
- Well-equipped labs with experimental and computational facilities

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- A pleasant work climate and collegial atmosphere in an international and interdisciplinary research team.
- Weekly (at least) contact with your colleagues and supervisors to share your knowledge, discuss the problems you might have, and collaborate on a solution.
- Optional social activities are typically organized by the team members and supported by the lab.
- You will be allowed to travel abroad (conferences) to communicate your scientific breakthroughs.
- A huge training offering (Doctoral Schools) that supports you during your PhD and prepares you for your future career.
- Bicycle allowance, benefits regarding public transport.
- Above all we offer you a Ph.D. degree with very good credentials for future employment.

Fellowship: ~ € 27.000 net per year including health insurance and other social security benefits.

More information:
https://www.ugent.be/phd/en
https://www.ugent.be/nl/jobs/personeelsvoordelen.htm