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| Supervisor(s) Prof. Mark Saeys | Period 4 years | Funding VLAIO |
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Full-time, funded PhD position: Computational catalysis for CO₂ to CO conversion during propene synthesis.

Aim

Modelling-guided design of catalysts for a retrofittable catalytic solution to decrease the CO₂ intensity of propane dehydrogenation through coupled CO₂ to CO conversion

Justification

Propylene is one of the key building blocks for the chemical industry, but divergent evolutions in the industry have given rise to the so-called “propylene gap”. To bridge this gap, on-purpose propylene production has been coming online. However, the on-purpose production is energy intensive and results in significant CO₂ emissions. To reduce their CO₂ intensity, a modification to existing plants is proposed that introduces oxidative dehydrogenation of propene (ODHP) coupled to CO₂ conversion to CO through innovative catalysis.

In a materials screening performed by the collaborating group of prof. Michiel Dusselier (KU Leuven), we found that V-CHA materials with particularly targeted properties are highly active and selective for this reaction. However, the molecular fundamentals of the mechanism and the catalyst are unknown. To develop and design the improved catalysts, in depth research is required. This involves mechanistic testing, spectroscopic characterization, and general hypothesis testing on synthesis – structure – activity relations. Several PhD students and post-docs, both at KU Leuven and UGent will work together on this challenge.

In your PhD research you will tackle the computational catalysis side of the research, evaluating relevant cluster models of vanadium catalysts (on zeolite or other supports) and investigating possible avenues for *in silico* catalyst design. You will investigate appropriate catalyst structures, reaction intermediates, and mechanisms, and support the characterization efforts of your colleagues through simulations. Your work will start from an ongoing thesis project that explores appropriate computational methodologies for investigating vanadium 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 CO₂-ODHP reaction using advanced computational catalysis tools.
- You will support the interpretation of experimental results obtained by your project colleagues at KU Leuven and at UGent
- You will assist the research group with limited educational tasks in topics related to your research.

LABORATORY FOR CHEMICAL TECHNOLOGY

Technologiepark 125, 9052 Gent, Belgium

Advisor

- Prof. [Mark Saeys](#)

Funding

Vlaio

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
- You work independently and have a strong feeling of responsibility both for you project and for lab safety
- A good proficiency in English (oral and written)

How to apply and application process

Apply before 1 October 2023 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 (starting date ideally asap, 1 January 2024 at the latest) and is open until the vacancy is filled. The position is not open for post-docs.

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 CO₂ 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/personneelsvoordelen.htm>