GHENT UNIVERSITY

CENTER FOR MOLECULAR MODELING

Ph.D. position available in the field of

Catalysis for the conversion of biomass compounds to platform chemicals.

The research group of prof. Van Speybroeck, embedded within the multidisciplinary **Center for Molecular Modeling** at **Ghent University, Belgium** (CMM, http://molmod.ugent.be), is looking for a highly motivated researcher to perform state-of-the-art research in the field of **theoretical modeling** of catalysis in **complex reaction environments**. We especially welcome candidates with a strong track record who may become eligible to apply for a prestigious Ph.D. fellowship at our national funding agency (FWO).

More info about the CMM

The CMM groups about 40 researchers of the faculties of Science and Engineering and Architecture with molecular modeling interests and is unique in the university as it clusters researchers with various backgrounds, from various departments and faculties. The CMM aims **to model molecules, materials and processes at the nanoscale by bringing together physicists, chemists, (bio-)engineers and stimulating collaborations across disciplines**. This multidisciplinary collaborative mission is the DNA of the CMM and key to achieve scientific excellence in the field of molecular modeling.

The CMM focuses on frontier research in six major areas: chemical kinetics in nanoporous materials, computational material research on the nanoscale, spectroscopy, many-particle physics, model development and bio- and organic chemistry. The six areas define the core-business of the main activities, and research in each of them is performed within the frame of a strong network with partners at Ghent University, in Flanders and at an international level. The research of this Ph.D. position is situated in the **"Nanoporous Materials"** research area, however to pursue excellence we strongly stimulate interactions between the various researchers in our team as well as with our vast network of national and international partners. The research of the CMM is internationally regarded to be at the forefront in its field.

The prospective candidate will join a **strongly connected research team** and will collaborate with national and international academic partners. He/she will benefit from the experience present in the research group to model chemical transformations at operating conditions. A strong body of expertise was developed in this area in the framework of various ERC grants.

More info about the research topic

This is a position within the framework of a joint **Excellence Of Science** project (EOS, https://www.fwo.be/en/fellowships-funding/research-projects/eos-research-project/) in collaboration with Prof. Bert Sels (KULeuven), Prof. Bert Maes (UA), Prof. Gwilherm Evano (ULB) and Prof. Christophe Detrembleur (ULiège). In this project named the **BioFactory** (Understanding and prediction of lignin-derived compound conversion in complex reaction environments for the production of fine chemicals and bio-based polymers) we aim to develop **new and green synthetic methodologies** for the transformation of the 4-lignin-derived monomers, obtained from an established and efficient lignin-first biorefinery process, into bulk/fine chemicals and polymers. Conversion of non-edible biomass to valuable functionalized chemicals and high-energy density fuels plays an important role in the transition to a non-fossil-based economy. Within this project you will work on **modelling activation energies**, reactivity patterns and screen for catalysts, ligands and directing groups for C-H and C-O activations. Furthermore, you will be at the front line of unravelling polymerization chemistry of recently developed cyclic(imino)carbonates. Because the scope of the BioFactactory is both to produce platform molecules and to use them for the production of industrially relevant compounds starting from lignin-derived monomers, the problems you will tackle vary both in size and in complexity. Modeling is quintessential to unravel

mechanistically the new synthetic routes and optimize selectivities. However, the proposed pathways take place in a complex molecular environment such as hot-pressurized water for the conversion of ferulic acid to bio-catechol (Bomon et al., 2019: https://doi.org/10.1002/anie.201913023). Therefore, you will use a rich plethora of modeling techniques which allow to obtain mechanistic insight at operating conditions, thus at the experimental temperatures and pressures and taking into account realistic solvents. Often we start using **density functional theory calculations** to gain fundamental understandings of the problems at hand. However, as computational power keeps increasing we are now able to model these systems within a more realistic environment e.g. the solvent environment and/or the realistic catalyst, … To this end free energy profiles can be constructed accounting for the operating conditions, using **advanced molecular dynamics methods**. Such techniques allow following chemical transformations in-situ, thus closely mimicking the experimental conditions. You will focus mainly on reactions in the field of organic chemistry in a homogeneous environment, ranging from reactions catalysed by organo- and transition-metal catalysts to reactions in complex solvent environments such as hot-pressurized water. Within the project the candidate will work in close collaboration with our experimental partners of the BioFactory project with whom we have already produced high impact publications. Our collaborative efforts within the experimental network, recently gave rise to very high impact papers in the broad field of chemistry (Bomon et al., 2019: https://doi.org/10.1002/anie.201913023; Ouhib et al., 2019: 10.1002/anie.201905969]

Who are we looking for?

We are looking for a highly motivated and creative Ph.D. candidate with:

- An excellent master's degree of an international equivalent in the field of Chemistry, Chemical Engineering, Physics, Physical Chemistry or a related field;
- A strong interest in molecular modelling;
- Excellent research and scientific writing skills;
- Perseverance and an independent, pro-active working style;
- The willingness to look beyond the borders of his/her own discipline and a strong motivation to work in a multidisciplinary team;
- Experience with quantum chemistry software (Gaussian, VASP, CP2K,…) and coding (Python, C, ...) is an advantage.
- Excellent collaboration and communication skills (written and verbally) in English

What can we offer you?

The selected candidate will get the ability to strengthen his/her CV within the context of a strongly motivated and multidisciplinary research team and have to ability to **contribute to challenging topical research** to solve important societal questions. He/she will have the opportunity to attend various international **conferences** and to include research stays abroad in the most prominent international research teams in this field within the framework of his/her Ph.D. The successful candidate will end up in a University with a strong **PhD community** that offers a broad range of **training possibilities** for PhD candidates, both within the research topic and focused on transferrable skills (e.g. time management, presentation skills, leadership, etc.).

How to apply?

It is the intention to fill this position as soon as possible. Students who will obtain their Master degree in June/July are also eligible. For more information on the position or the CMM, candidates can get in touch with Prof. Veronique Van Speybroeck (Veronique.vanspeybroeck@ugent.be).
Interested candidates are requested to prepare the following documents:

1. The filled out application form (see Application-Form.doc)
2. A motivation letter
3. A curriculum vitae
4. Copies of the relevant diplomas and grade lists

All these documents should be send to cmm.vacancies@ugent.be, according to the guidelines mentioned in the application form.