

Open Research Positions (Ph.D. and postdoc level)
in the research group of prof. V. Van Speybroeck
at the Center for Molecular Modeling, Ghent University, Belgium

Within the framework of various running and recently granted projects various research positions are available.

Topics of the research positions :

- **Modeling Metal Halide Perovskites for next generation optoelectronic applications** – Intended for applicants with a physics (engineering) background

Within the framework of an interuniversity projects with experimental partners of the KULeuven (Prof. Hofkens, Roeyfaers), UAntwerpen (Prof. Bals, Van Aert, Verbeeck). Also joint PhDs with KULeuven, UAntwerpen are possible where partly experimental work is performed.

- **Zeolite catalysis for the conversion of new feedstocks (CO₂, C₁ chemistry, methanol conversion)** – Intended for applicants with a chemical (engineering) background

Within the framework of national/international large scale research projects with partners at KULeuven, Utrecht University, University of Oslo, University College London, KAUST – Saudi Arabia,... International exchanges with the partners are possible

- **Hybrid membrane/sorption technology for more efficient C₂ and C₃ separations** – Intended both for applicants with a chemical, physics (engineering) background

Within the framework of a CO₂ Moonshot project with partners of the KULeuven (Prof. Vankelecom, Ameloot), VUB (Joeri Denayer) and with an industrial advisory board

- **Design of materials to capture and convert energy molecules (H₂)** – Intended for applicants with a chemical or physics(engineering) background

Within the framework of a CO₂ Moonshot project with partners of KULeuven, VUB, UAntwerpen

More info about the research within the Van Speybroeck group

The research group of prof. Van Speybroeck is embedded within the multidisciplinary **Center for Molecular Modeling** (CMM, <http://molmod.ugent.be>) and has received **world recognition for modeling functional nanoporous materials with applications in sustainable chemistry, nanosensing and clean energy**. We acquired a unique position worldwide, as we model materials as close as possible to experimental conditions. To this end we are continuously developing and applying the most advanced models that allow to bridge from the nanoscale to the experimentally observed length and time scales. Within the framework of the currently opened positions we aim to develop machine learning potentials, coarse grained models to model materials at realistic length scales up to 1 μm . Furthermore for the chemically oriented topics we will rely on our vast expertise in molecular dynamics methods to simulate catalytic processes at operating conditions, e.g. at realistic temperatures, pressures, within solvents, ... Our team consists of a broad variety of researchers, some of them are performing more theoretically oriented research where new methods are developed, implemented in software packages whereas other researchers use available programs and focus on the application oriented research questions.

Importance of the research

Our society is confronted with important challenges, such as how can we provide an affordable and clean energy system without endangering future generations, how can we protect our limited natural resources, how can we combat environmental pollution, how can we mitigate climate change. Functional nanomaterials play a pivotal role in the development of future technological solutions to provide answers to these questions. From a purely experimental basis, it is extremely difficult to establish a causal relation between nanometer scale structural modifications and the observed macroscopic function of the material. Modeling functional nanomaterials in close synergy with experimental groups has the potential to give this nanoscopic insight, provided it yields a realistic nanometer scale representation of the functional material. As we are modeling realistic materials and processes we are actively participating in collaborations with experimental partners and with industry.

More info about the Center for Molecular Modeling

The Center for Molecular Modeling (CMM), headed by Prof. Van Speybroeck, is a multidisciplinary research center, which groups about 40 researchers of the faculties of Science and Engineering and Architecture with molecular modeling interests. The CMM aims to model molecules, materials and processes at the nanoscale by bringing together physicists, chemists, (bio-)engineers and stimulating collaborations across disciplines. Within the CMM collaborative research between researchers with various backgrounds and from various departments is pursued. This multidisciplinary collaborative mission is the DNA of the CMM and key to achieve scientific excellence in the field of molecular modeling.

Who are we looking for?

- You are highly motivated to become an independent researcher and to contribute to important societal problems related to clean energy production, non-fossil based production of chemicals, design of materials for the next generation energy carriers,...
- You have a strong academic record showing your potential to become an excellent researcher.
- You have excellent communication skills and have a strong motivation to collaborate both within the CMM with other researchers and with other researchers of our network.
- For PhDs : You have or will soon obtain your master's degree in the field of Chemistry, Chemical Engineering, Physics, Physical Engineering.
- For postdocs : You can rely on a CV with a strong track record based on high profile papers, contributions to international conferences,....
- We are looking for candidates with a pro-active working style; 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 for prospective PhD students and a requirement for prospective postdocs. For PhD student without modelling experience we will provide active training during the first months.

What can we offer you?

- You will work in a highly motivated and dynamic team, will be actively trained by various researchers of the team that consists of **various junior and senior researchers** with different backgrounds.
- You will have the ability to participate actively in various international conferences, perform international research stays at the most prominent universities worldwide with whom we collaborate to strengthen your skills.
- Interested candidates will have the ability to also contribute to education of the CMM by giving exercise classes.
- Van Speybroeck has a very strong track record in coaching PhD students, under her supervision 32 successful PhD candidates were performed. Most of them found jobs afterwards in industry, academia and have built very strong CVs during their time at the CMM.
- Depending on your interests we will define a research topic that fits your interests, which is more oriented towards theoretical model development, programming, solving application oriented questions with our experimental and industry partners.

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. Interested candidates are requested to prepare the following documents:

1. The filled out application form that can be found on our website
2. A motivation letter, including the preferred research topic
3. A curriculum vitae
4. Copies of the relevant diplomas and transcript (certified record of full enrollment history at educational school). Diplomas and transcripts that are not in Dutch or in English should have an official translation in Dutch or English.
5. List of publications

The files should be saved as PDF and named as follows:

- [File number as listed above]_[Your name] _Application_ 2021_PHD for the PhD Fellowships
- [File number as listed above]_[Your name] _Application_ 2021_POST for the Postdoctoral Fellowships

All these documents should be sent to cmm.vacancies@ugent.be with the vacancy number in the subject (2021_PHD or 2021_POST), according to the guidelines mentioned in the application form.