GHENT UNIVERSITY

CENTER FOR MOLECULAR MODELING

Ph.D. position available in the field of

Modelling C1 catalysis in nanoporous zeolite materials at operating conditions to convert new feedstocks

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 **nanoporous zeolite materials**. 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 PhD research will focus on modelling C_1 catalysis in nanoporous zeolite materials. **C_1 catalysis** – the conversion of one-carbon molecules such as CO_2, CO, CH_4, CH_3OH into high-value platform chemicals and liquid fuels – has attracted widespread attention in the quest for reducing anthropogenic greenhouse gas emissions. The conversion of non-fossil feedstocks like biomass as well as to recycle CO_2 into high-value chemicals, requires the design of next generation multifunctional catalysts which are highly selective and also robust in a broad operation window. In general, the activation of thermodynamically stable C_1 molecules like CO_2 and their transformation to olefinic and aromatic products, the main building blocks of the chemical industry, is highly challenging. Thanks to their specific porous nature, **zeolite materials** will play a prominent role in the **conversion of C_1 compounds**. A thorough understanding of the persistent intermediates and governing reaction mechanisms is essential to improve the catalyst efficiency and selectivity. More specifically, for the conversion of CO_2 into hydrocarbons, the precise mechanism for C-C bond formation and the role of the presence of CO, CO_2, H_2 and

H_2O in the reaction environment are so far improperly understood. Nevertheless, such fundamental insight is still lacking. To this end, **computational modeling** can prove a powerful method to aid in the understanding of the process and the design of next-generation multifunctional catalysts. In this **Ph.D. research**, you will systematically investigate C-C coupling reactions in the presence of CO, H_2 and H_2O for a variety of process conditions. Various reactions are closely related to the mechanisms found within the Methanol-to-hydrocarbons (MTH) process. Therefore, several aspects of the conversion of CO_2 and CH_3OH species on different zeolite catalysts will be investigated using a large set of modeling techniques. By applying a combination of **molecular dynamics (MD) simulations and density functional theory (DFT) calculations**, you will perform a mechanistic study on the role of CO_2 in these processes, taking into account the complex molecular environment and actual reaction conditions. The research topic will be conducted in close collaboration with excellent experimental groups to guide the design toward new and promising functional materials. Several collaborative research papers which illustrate our efforts in this area (CO_2-to-hydrocarbons and methanol to hydrocarbons) are cited below.[1–4]

(1) Ramirez, A.; Dutta Chowdhury, A.; Dokania, A.; Cnudde, P.; Caglayan, M.; Yarulina, I.; Abou-Hamad, E.; Gevers, L.; Ould-Chikh, S.; De Wispelaere, K.; Van Speybroeck, V.; Gascon, J. Effect of Zeolite Topology and Reactor Configuration on the Direct Conversion of CO2 to Light Olefins and Aromatics. *ACS Catal.* **2019**, *9* (7), 6320–6334.

(2) Yarulina, I.; Wispelaere, K. D.; Bailleul, S.; Goetze, J.; Radersma, M.; Abou-Hamad, E.; Vollmer, I.; Goesten, M.; Mezari, B.; Hensen, E. J. M.; Martínez-Espín, J. S.; Morten, M.; Mitchell, S.; Perez-Ramirez, J.; Olsbye, U.; Weckhuysen, B. M.; Speybroeck, V. V.; Kapteijn, F.; Gascon, J. Structure–Performance Descriptors and the Role of Lewis Acidity in the Methanol-to-Propylene Process. *Nat. Chem.* **2018**, *10* (8), 804.

(3) De Wispelaere, K.; Wondergem, C. S.; Ensing, B.; Hemelsoet, K.; Meijer, E. J.; Weckhuysen, B. M.; Van Speybroeck, V.; Ruiz-Martínez, J. Insight into the Effect of Water on the Methanol-to-Olefins Conversion in H-SAPO-34 from Molecular Simulations and in Situ Microspectroscopy. *ACS Catal.* **2016**, *6* (3), 1991–2002.

(4) Westgård Erichsen, M.; De Wispelaere, K.; Hemelsoet, K.; Moors, S. L. C.; Deconinck, T.; Waroquier, M.; Svelle, S.; Van Speybroeck, V.; Olsbye, U. How Zeolitic Acid Strength and Composition Alter the Reactivity of Alkenes and Aromatics towards Methanol. *J. Catal.* **2015**, *328*, 186–196.

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.